Microstructure Modeling in Aluminum - Scandium Alloys

Master Thesis

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by

René Wang

0930800

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STATUTORY DECLARATION

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Date René Wang

Preface

First of all, I am very thankful to my first supervisor Univ.-Prof. Dipl.-Ing. Dr.techn. Bernhard Sonderegger and my second supervisor Dipl.-Ing. Dr.techn. Johannes Tändl. I also want to mention the scientific and non-scientific personnel at the Institute of Material Sciences, Joining and Forming, who supported me while working on my master thesis. I am also grateful to my parents, who made it possible for me to study at the Technical University of Graz. In particular, I want to thank my girlfriend, who supported me during my studies and also took care of me in stressful times. Last but not least, I want to thank my colleagues and friends, with whom I spent many long evenings learning and preparing for exams.

René Wang, February 2017

Abstract

In this master thesis, the thermodynamic and diffusion databases for the precipitation kinetic simulations in the software-program MatCalc for Al-Sc alloys were first evaluated and then optimized. The evaluation of the standard thermodynamic database was performed through equilibrium phase diagram modeling, which resulted in a not well placed diagram. After changing specific parameters to adjust the equilibrium phase diagram and the thermodynamic database, precipitation kinetic simulations were performed. The simulations were first executed with the modified thermodynamic database and the standard values of the diffusion database. Then, the outputs, e.g. precipitate radii, volume fraction and number density, were compared and evaluated with literature data and if necessary, changes of the diffusion database were made, to optimize it. This led to an accurate simulation model for precipitation kinetics in the Al-Sc alloy system.

Keywords: Al-Sc alloys; precipitation-kinetics; MatCalc

Content

List of Abbreviations

Al	Chemical element Aluminum
Mg	Chemical element Magnesium
Sc	Chemical element Scandium
Zr	Chemical element Zirconium
Al_nSc_m	Intermetallic phases of Aluminum and Scandium
Al-Ti	Aluminum-Titanium alloy
Al-Ti-B	Aluminum-Titanium-Boron alloy
Al-Ti-C	Aluminum-Titanium-Carbon alloy
CALPHAD	CALculation of PHAse Diagrams
H	Hardness
Rn	Roundness
CNT	Classical Nucleation Theory
eq.	Equation
LSW	Lifshitz-Slyozov-Wagner
SFFK	Svoboda-Fischer-Fratzl-Kozeschnik
GBB	Generalized Broken Bond
NNBB	Nearest-Neighbor Broken Bond
NKW	Numerical Kampmann Wagner
FCC_A1	Code for Al-matrix crystal system as used in CALPHAD-database
r_v_mean	Mean precipitate radius (volume weight)

1. Introduction

Aluminum (Al) and its alloys find applications in several fields, such as sports, electronics, aerospace, automotive and packaging industries. Fulfilling the demands in the different application fields, it is necessary to add other elements to Al, like magnesium (Mg), scandium (Sc), zirconium (Zr) etc., alone or in combination. The presence of alloying elements, improves properties such as specific strength and stiffness, workability, weldability, corrosion resistance, hardness and optimizes the microstructure of the material. [1]

Especially in the aerospace industries, Al-alloys are widely used materials. The mainly used Al-Cu-Mg alloys have high strength, but bad corrosion resistance and weldability. An important alloying element for Al in this industry, will maybe Sc in the future, which has better corrosion resistance. [1] Its Al_3Sc-precipitates are fine distributed in the microstructure and Sc also acts as grain refiner [2]. Both properties lead to an increase of the yield strength, shown in Figure 1. Further properties will be treated in more detail in the chapter literature review. The modifications on Al initiated by Sc, fit perfectly to the demands in the aerospace industries.

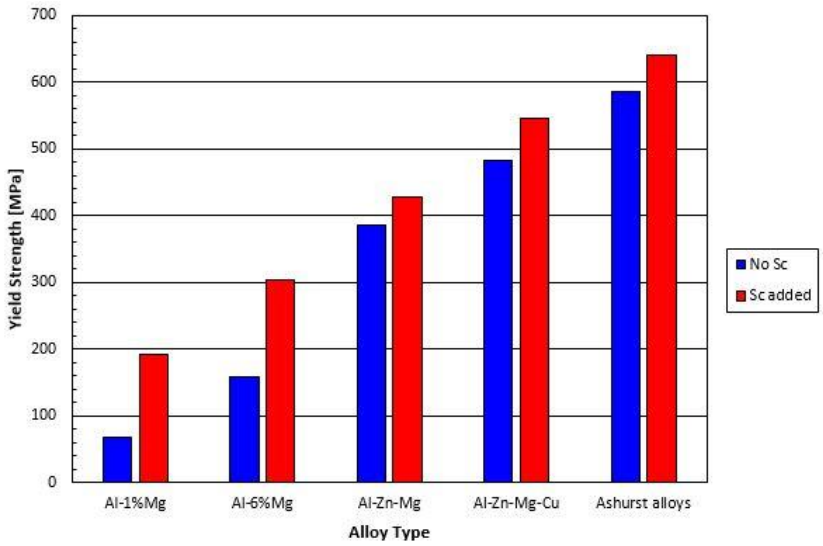

Figure 1: Yield strength increase by Scandium [3]

Additional to the different possible alloy compositions, there are several heat treatments possible. Different temperatures, heating/cooling rates, holding times and sequences, influence the alloy and lead to multiple possibilities, e.g. the microstructure appearance of the alloy and which properties it has.

Choosing the right alloy for an application, it is necessary to know the above mentioned properties. It is evident, that for one specific alloy a number of specimens with different compositions and experiments are needed to gather information. Avoiding this expensive and time consuming procedure of specimen production as well as preparation and analysis, it is useful to simulate the kinetics of the microstructure.

For this purpose, MatCalc is a helpful program with an uncomplicated graphical user interface, which serves different thermodynamic and kinetic simulations. It is based on the CALPHAD-method, which includes most of the thermodynamic parameters for describing the Gibbs Free Energies of an alloy system. The application includes thermodynamic equilibrium calculations, precipitation kinetics and discrete microstructure simulations, based on three theoretical models [4]:

- Multi-component extension of classical nucleation theory.
- Powerful model for the growth of precipitates in multi-component multi-phase environment.
- Complete treatment for interfacial energies between precipitate and matrix.

Focus of this thesis is the investigation and if necessary, the optimization of the existing Al-alloy thermodynamic and diffusion database to meet the reference values from experimental and simulation data.

2. Literature Review

This chapter contains an overview of the Al-Sc system and the pure elements in the first part. The second part gives an overview of the models which MatCalc uses. At the end of this section MatCalc is described in more detail and an outline is given on how it works.

2.1 Material

At the beginning of this section, the properties of the pure elements are regarded, to get a feeling about the effects of Scandium in Aluminum. Furthermore, the properties and the microstructure appearance of different Al-Sc alloys are described.

2.1.1 Aluminum

Aluminum is after steel the most used metal. Based on the diversity of the properties and the possibility to combine them, it can be used in different application areas. In 2015 nearly 79 billion of tons of Al were consumed, which is almost four times the amount of 2001. [5] [6]

The raw material used for aluminum production is bauxite, which is transformed to Al-oxide in the Bayer process. Afterwards, the Al-oxide is transformed by an electrolytic process to pure Aluminum. [5]

Aluminum is a silver-white metal and its shiny surface has a high reflectivity for light, heat and electromagnetic radiation. Pure Al has a density of 2,6989 kg/dm^3 and is therefore categorized as light metal. It has a face-centered cubic structure with a space filling of 74 % and a lattice parameter of 0,40496 nm. Due to the face-centered cubic structure, it is well deformable in cold and hot work processes. The melting point is at 660,2 °C and the heat conductivity and electric conductivity is 235 W/mK and 37,67 m/Ωmm^2, respectively. The Young's modulus is 66,6 GPa and the modulus of shear is 25 GPa, as well as mechanical properties are the yield strength of 17 MPa and the tensile strength of 45 MPa. [5]

2.1.2 Scandium

Sc is also a silver-white metal, which was discovered by L. F. Nilson at Uppsala, Sweden in 1879. The name originates from the latin word "Scandia", because the mineral euxenite, in which Nilson found Sc first, was not found outside of Scandinavia at this time. Meanwhile the metal was found in more than 800 mineral species in small amounts all over the world and is more common in the earth's crust than lead. Sc is not explicit produced, it is a byproduct that occurs during the processing of different ores. [7]

Its density is about 2,99 kg/dm^3 and belongs therefore also to the light metal group. Sc has a hexagonal close packed crystal structure and its melting point is at 1541 °C. The Young's modulus is 79,3 GPa and the shear modulus is 44,2 GPa. The thermal conductivity is lower than from Al, with 15,8 W/mK. [3]

2.1.3 Aluminum – Scandium alloys

If Sc is added to Al, it acts as a dispersoid strengthener, grain refiner, and recrystallization inhibitor. It reduces the possibility of hot cracking during welding and has positive effects on the weldability and welding properties. [2]

Sc-contents with up to 1 wt.% at heat treatments between 250 °C to 350 °C lead to extensive precipitation hardening. It is one of the most effective precipitation hardener element and has a higher strengthening effect than Zr in Al. Smaller Sc-contents, with up to 0,8 wt.%, improves the properties and mechanical strength of an Al-alloy, as mentioned in Figure 1. Al-alloys with up to 2 wt.% Sc in as-cast state and homogenized state have a strength increase of 50 MPa and 80 MPa, respectively. For wrought alloys with Mg and a small amount of Sc (≤ 0,35 wt.%) it is even possible to reach a strength increase of 100 – 200 MPa. [8]

Sc in hypereutectic additions (> 0,55 wt.%) to Al-alloys forms fine equiaxed structures, with sizes between 25 – 50 µm and acts as a stronger inoculant compared to Al-Ti, Al-Ti-B and Al-Ti-C master alloys [8].

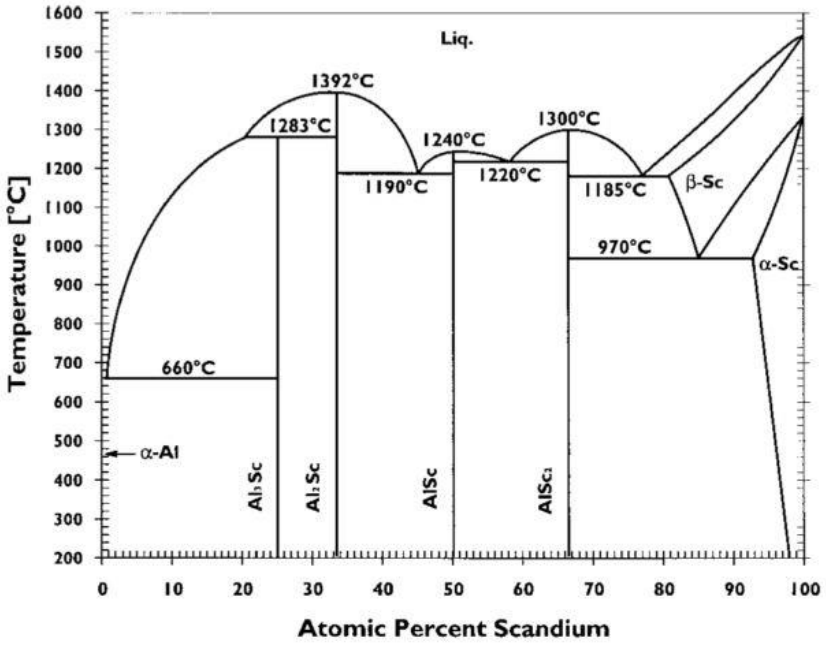

Figure 2: Al-Sc phase diagram [9]

Dependent on the composition, the Al-Sc system forms four equilibrium intermetallic phases (Al_3Sc, Al_2Sc, AlSc, $AlSc_2$), as shown in Figure 2. The important region, this thesis focuses on, is illustrated in

Figure 3. It displays that only the Al_3Sc intermetallic phase will be formed at this Sc concentrations, where an eutectic reaction takes place at 0,55 wt.% Sc and 655 °C, with the maximum solubility of Sc in Al is 0,4 wt.%. [9]

A detailed view of the solvus line is plotted in Figure 4. It is evident that Sc is not soluble in Al at room temperatures and therefore the Al_3Sc precipitates are formed.

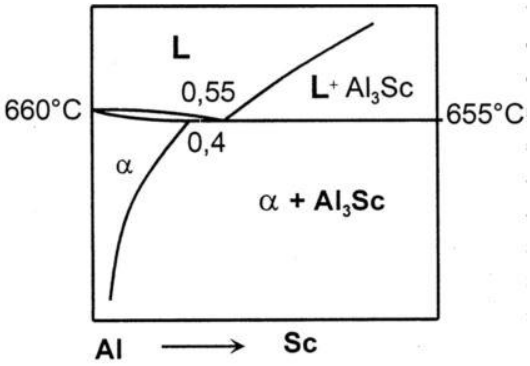

Figure 3: Al-rich region of Al-Sc phase diagram [10]

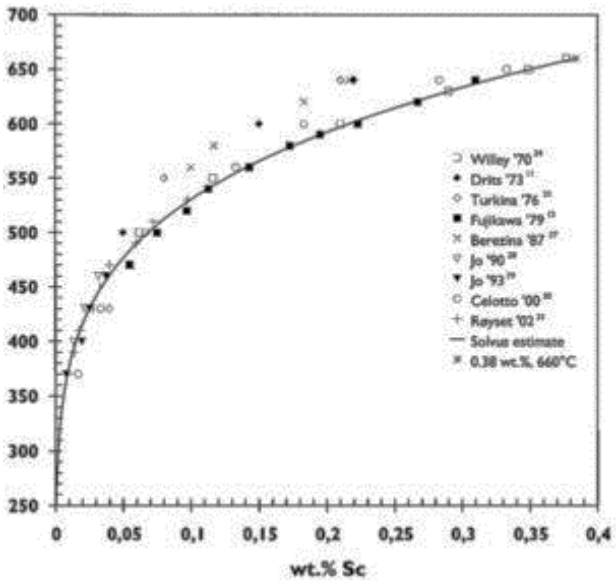

Figure 4: Solubility of Sc in Al [9]

2.1.3.1 Al_3Sc phase

The Al_3Sc phase, formed in Al-Sc alloys, has a $L1_2$-structure with a lattice parameter of 0,4103 nm, compared to Al (0,40496 nm), which results in a misfit of 1,33 % between Al_3Sc and the α-Al matrix at ambient temperature. In an Al_3Sc unit cell, the Sc-atoms are located at the corners and the Al-atoms take over the spaces on the cube faces, as illustrated in Figure 5. [11] [12]

The benefits of the Sc addition are strongly linked to the Al_3Sc phase, which can be formed in three different ways, depending on chemical composition and heat conditions during processing [13]:

1. During solidification after casting or welding: Precipitates nucleate in the melt and act as grain refiner, which requires a hypereutectic composition of more than 0,6 wt.% Sc.
2. High temperature processing in the range of 400 °C to 600 °C: Homogenization, hot rolling or extrusion leads to a dense distribution of the particles. This will not have a significant strengthening effect but a stabilizing effect on the grain structure.
3. Heat treatments in the range of 250 °C to 300 °C: Precipitation hardening occurs in alloys supersaturated in Sc.

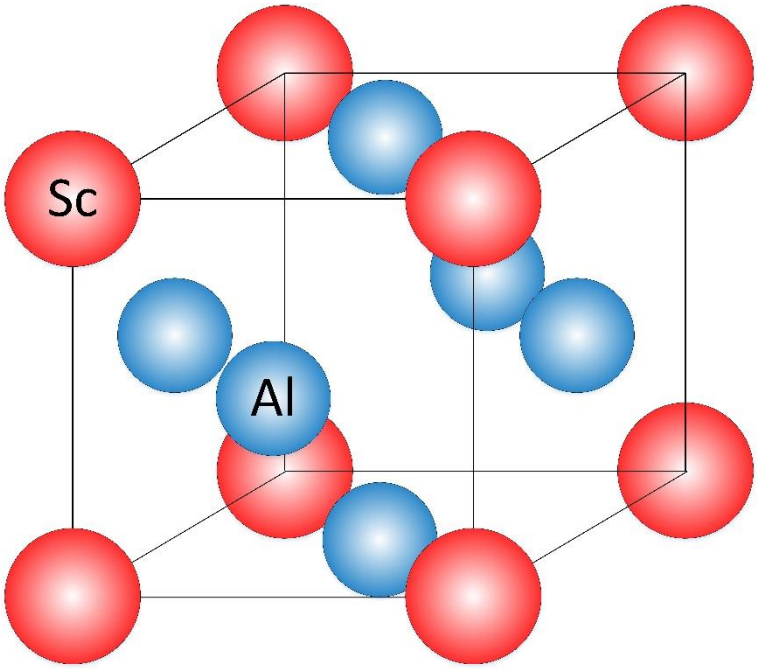

Figure 5: Face centered cube with its atomic arrangement of an Al_3Sc phase [9]

2.1.3.2 Scandium effects

V. Davydov and T. Rostova mentioned in an extensive review-paper three important effects of Sc in Al, which are listed in this section [10]:

The Antirecrystallization Effect

The addition of Sc increases the recrystallization temperature of an alloy in the most effective way. The high density of Al_3Sc dispersoid particles results in a high antirecrystallization effect. Due to the similarity of the crystal lattice of Al_3Sc particles and the α-Al matrix, the Al_3Sc phase precipitates homogeneously during the decomposition of the solid solution, with a very high density of spherical

particles. [10] In Figure 6 the increasing recrystallization temperature in respect to the concentration of different alloying elements is demonstrated.

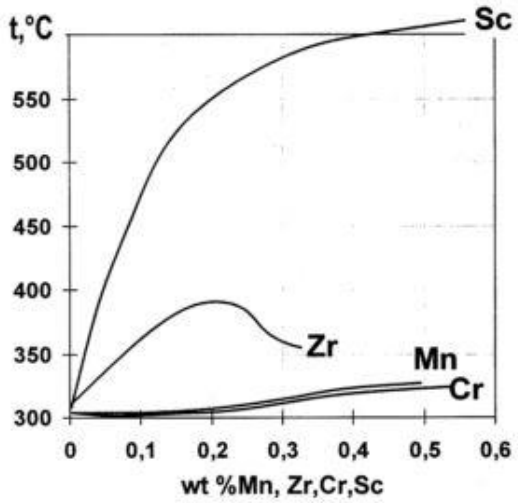

Figure 6: Recrystallization temperatures vs. concentration of different alloying elements [10]

The strengthening effect

The strengthening effect is caused by the high dispersity of the Al_3Sc dispersoids, shown in Figure 7. The curves of microhardness vs. annealing time at different temperatures of an Al-0,41 wt.% Sc alloy ingot with a diameter of 134mm are plotted in Figure 8, revealing a strong strengthening as a result of annealing. Microhardness of ingots in the as-cast state is about 350 MPa and after annealing it can increase up to 2,5 times. The curves suggest that Sc is in a supersaturated solid solution after the casting process and during annealing it comes to the formation of the dispersed Al_3Sc particles. The decrease of the microhardness is caused by coagulation of the strengthening Al_3Sc particles. [10]

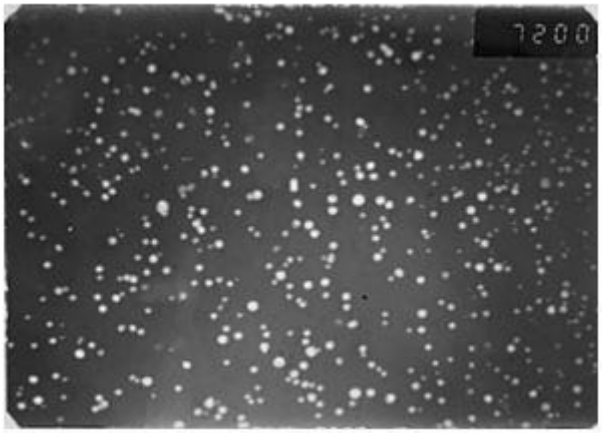

Figure 7: Al_3Sc phase particles formed during decomposition of Sc solid solution (Al-0,4 %Sc), (x72000) [10]

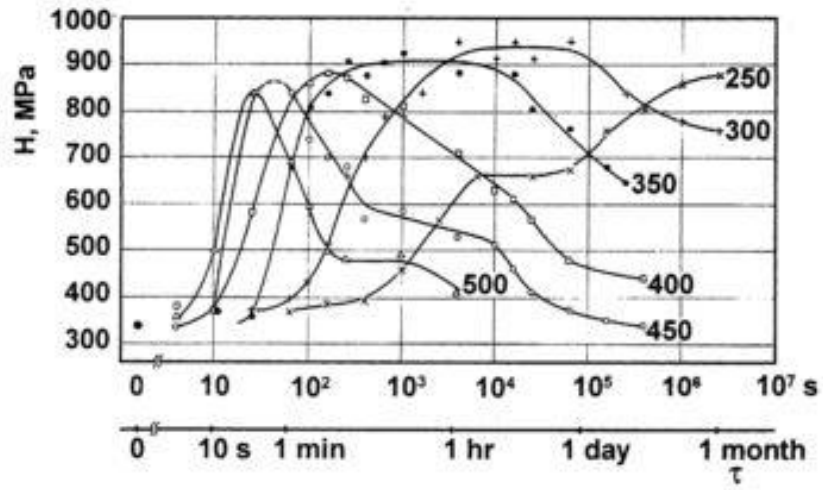

Figure 8: Microhardnesses at different annealing temperatures and times [10]

The modifying effect

The modifying effect of Sc describes the significant refinement of the dendritic structure [14]. The differences between a 5083 alloy without and with Sc are displayed in Figure 9. Commercial Sc-bearing Al-alloy ingots, continuously casted, have a nondendritic structure, which appears isotropic and shows geometrical equality of grains and the dendritic parameter [10]. Two more examples of this effect in a higher magnification, are illustrated in Figure 10 on the basis of the comparison of a 1970 alloy and a 1570 alloy.

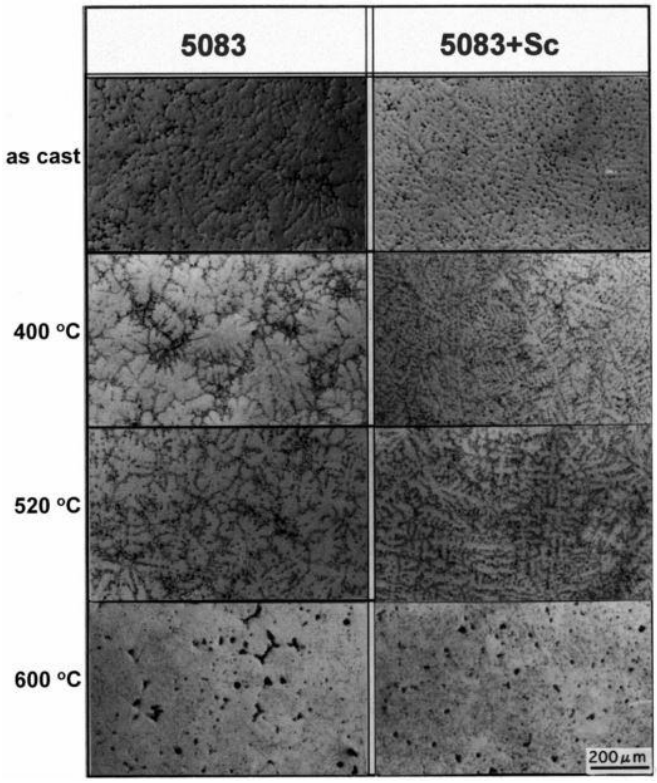

Figure 9: Differences of microstructures without and with Sc at various temperatures [14]

This strong modifying effect of Sc in Al-alloys is the result of two factors [10]:

- A large number of nuclei in the form of Al_3Sc particles in a unit of melt volume.
- A high effectiveness of the inoculate action of the Al_3Sc particles.

The modifying effect also appears in multi component alloys, like mentioned above in the 5083 alloy, and gets influenced by them. The presence of Zr in an Al-Sc alloy changes the modifying effect remarkably. If Zr is added, the modifying effect occurs already above 0,18 wt.% Sc, otherwise it appears above 0,55 wt.% Sc. [10]

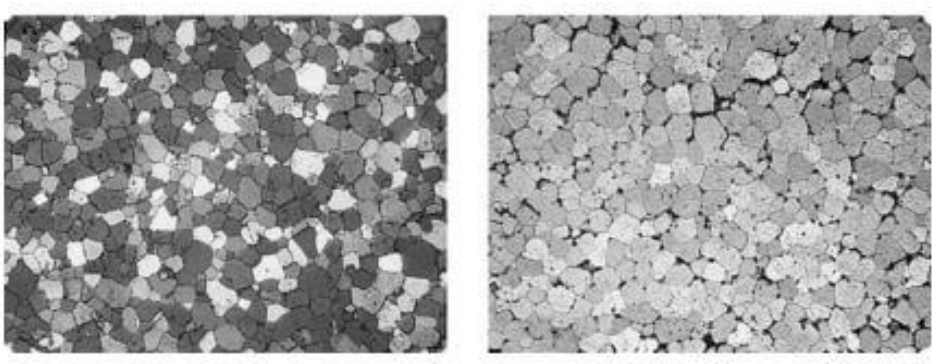

Figure 10: Nondendritic structure of a continuously cast 1970 alloy (left) and a 1570 alloy (right), both (x22000) [10]

2.1.3.3 Influences of Sc-concentration on microstructure

Here, the influence of Sc on the microstructure is discussed, where different Sc-concentrations lead to different microstructures appearances.

Unalloyed Al has large columnar grains with dendritic substructure, which reduces the workability, yield strength and ductility of the material. Figure 11a shows this regular microstructure of pure Al without any grain refiner. At a Sc content of 0,5 wt.% the microstructure changed to a coexisting of smaller columnar and equiaxed grains, than those of pure Al, as seen in Figure 11b. Figure 11c shows that an increase of Sc to 0,7 wt.% leads to a significant decrease in grain size and an enlargement of the roundness of the grains. The columnar grains disappeared completely and the equiaxed structure remains. A further increase of the Sc concentration brings no additional benefit in grain refining, as the structure of Al with 1 wt.% Sc in Figure 11d shows. [8]

Additionally, the influence of Sc on Al is plotted as function of the Sc content in Figure 12, to give a better overview.

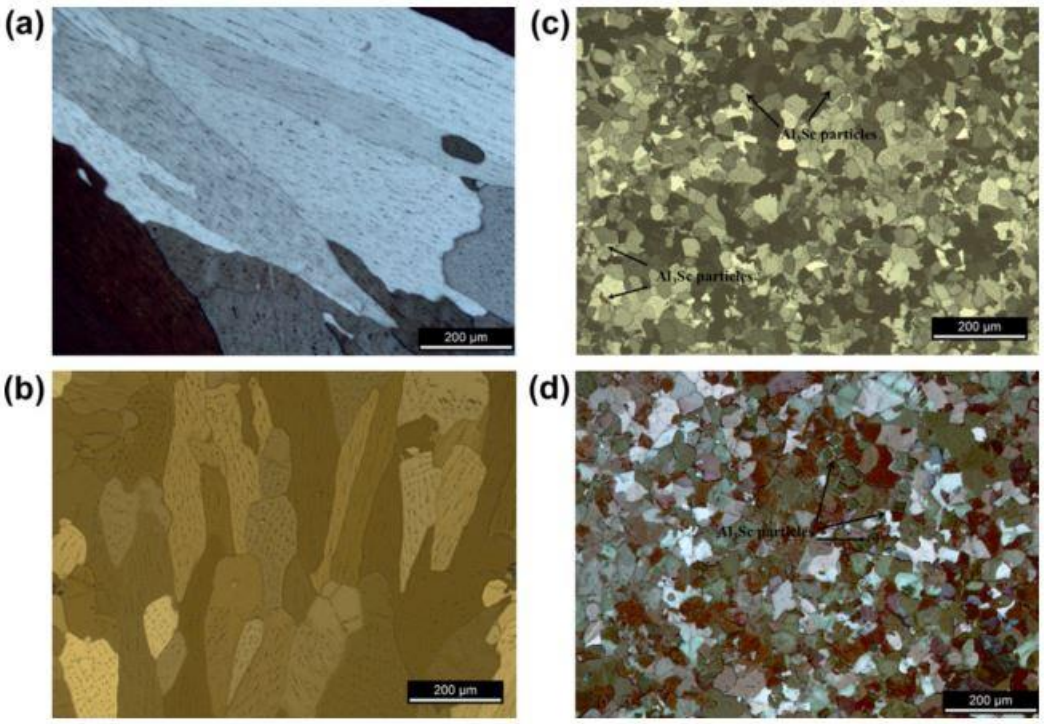

Figure 11: Low magnification optical micrographs of as cast (a) pure Al; (b) Al-0,5Sc; (c) Al-0,7Sc; (d) Al-1Sc [8]

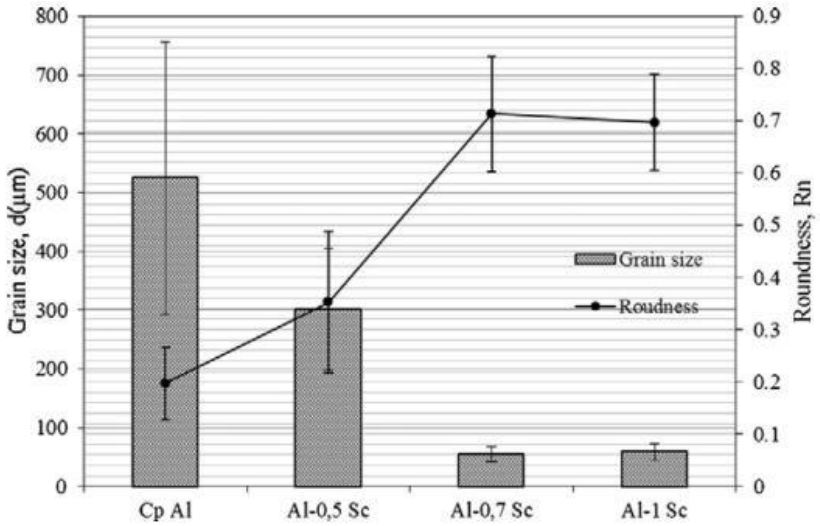

Figure 12: Functions of the Sc content, which shows the influence of Sc on the grain size and the roundness in Al-Sc alloys [8]

2.2 Precipitate evolution simulation

The formation of precipitates happens in three stages: nucleation, growth and coarsening. In this chapter the stages are described and mathematical methods for the simulation of this process are presented.

2.2.1 Nucleation

Basically, nucleation happens randomly and it is not possible to make a prediction on where and when nuclei will be formed. Therefore, nucleation is considered as stochastic process, which is strongly linked to an energy barrier. The higher this energy barrier, the higher must be the effort to overcome it. However, in precipitate nucleation processes this relation is not linear, a small increase of the energy barrier could lead to a stop of the nucleation. For that reason, this measure is an important quantity. [4]

To make nucleation possible, an attractive force between atoms forming the new phase is necessary, the so called driving force. A bigger driving force increases the probability of a single nucleation event and enhances the nucleation rate. [4]

The classical nucleation theory (CNT) has its origin from the treatments of the equilibrium between free surfaces of liquid and its vapor in a closed vessel, published by Sir W. Thomson in 1870 [15] and was further developed by M. Volmer and A. Weber [16] and R. Becker and W. Döring [17]. The fact that molecules in vapor and liquids are able to move freely in space, in contrast to solid material, where atoms move in discrete spatial portions, has to be taken in account and as well as other aspects which are important to consider in solid state nucleation [4]:

- The interface between a nucleus and the matrix phase is well defined, which can occur coherent, semicoherent or incoherent.
- Different molar volumes between the parent phase and the precipitate leading to a long range elastic stress, which usually impedes nucleation.
- Two kinds of nucleation: homogeneously in the undisturbed crystal lattice; heterogeneously at dislocations, grain boundaries, inclusions, etc.
- Elastic stresses can be relaxed by structural vacancies.
- Atom – vacancy exchange mechanism influences the nucleation.
- Atom – vacancy exchange diffusion is proportional to vacancy-density.
- Phases with identical chemical composition can form crystal structures with different structure complexity, which leads to a crystal structure selection.
- Temporary formation and dissolution of metastable precursor phases complicate the precipitation process.

The CNT does not take the previous mentioned points into account explicitly, but is an adequate model to describe the proceedings in the microstructure.

Nevertheless, CNT is a continuums-mechanical method, which considers the energy barriers or nucleation energies with Boltzmann statistics, to characterize the probability of forming supercritical nuclei [18].

2.2.1.1 Interface between matrix and precipitate

In solid materials, atoms move through the crystal lattice commonly through atom – vacancy exchange. According to this fact, the precipitate and the parent phase show some different crystallographic relationships. [4]

In Figure 13 two precipitates with coherent interfaces are shown, the left one has no volumetric misfit and the right has one. The precipitates have the same crystal structure, but above a critical size of the right precipitate the coherency cannot be maintained [19]. The continuity and periodicity of the lattice planes has a significant impact on the interaction between dislocations and the particle under mechanical load, which plays a big role in precipitation strengthening simulation. The volumetric misfit at the precipitate gets transferred to local atomic displacements, leading to a long range elastic stress field around the particle. [4]

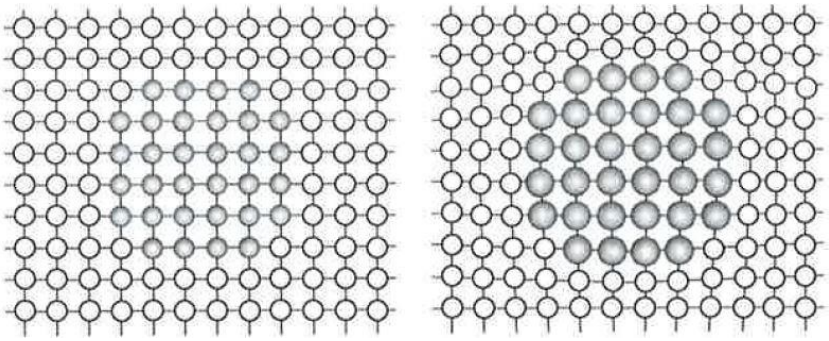

Figure 13: Schematic representation of a coherent precipitate without (left) and with (right) volumetric misfit [4]

Precipitates with semicoherent and incoherent interfaces are schematically plotted in Figure 14. The left figure shows a precipitate with a larger volumetric misfit as in Figure 13 (right), which results in a semicoherent interface on the bottom and top sides and an incoherent relationship on the left and right sides of the precipitate. Here a minimum of one atomic bond is broken, which also results in an introduction of elastic stress energy in the system. In the right plot, the crystal structure of the new phase is also indifferent and the orientation of the crystal structure misfits, which results in a fully incoherent precipitate. Such an incoherent particle is an ideal source and sink for vacancies, which leads to a rapid elastic stress relaxation. [4]

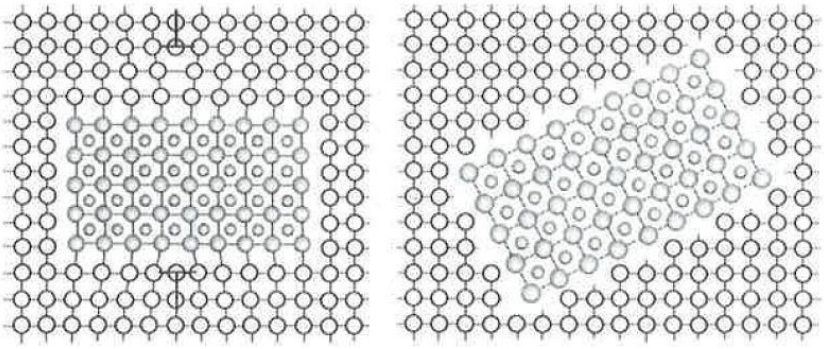

Figure 14: Precipitates with semicoherent ([left] bottom and top) and incoherent ([left] right and left sides; [right] all sides) interfaces [4]

2.2.1.2 Free energy of nucleus formation

This section describes the change of the total free energy in relation to the forming event of a single nucleus.

First, it is important to consider, that every single nucleation event randomly occurs by heterophase fluctuations. This means that the basis of nucleation in CNT consists of microscopic fluctuations in a macroscopic homogeneous and equilibrated system of constant energy with no composition gradients around a nucleus. Second, a small amount of matter is transferred, so that the thermodynamic properties of the matrix are not changed, which implies that the number of molecules for nucleation is big enough and the energy in the system remains constant. [4]

In Figure 15 some clusters of molecules of the precipitate phase β in the parent phase α are illustrated. A cluster with critical radius is shown in the dashed circle, all other clusters have subcritical radii. [4]

Assuming that the formed nucleus is spherical in shape, the change of the total free energy can be written as

$$\Delta G_{nucl} = \frac{4}{3}\pi\rho^3 \cdot \Delta G_{vol} + 4\pi\rho^2 \cdot \Delta G_{surf}, \qquad \text{eq. 2.1}$$

where ΔG_{vol} is the specific volume free energy change for transforming a volume unit of the parent phase into precipitate phase, ΔG_{surf} is the required energy to build a unit area of precipitate - matrix interface, which is equal to the interfacial energy γ, and ρ denotes the radius of the cluster. Furthermore, the ΔG_{vol} can be separated to

$$\Delta G_{vol} = \Delta G_{vol}^{chem} + \Delta G_{vol}^{el}, \qquad \text{eq. 2.2}$$

where ΔG_{vol}^{chem} is the chemical and ΔG_{vol}^{el} is the mechanical contribution. The chemical contribution can be identified as the chemical driving force, calculated with

$$d_{chem}^{\beta} = \sum_i X_i^{\beta} \mu_i^{\alpha} - g^{\beta}. \qquad \text{eq. 2.3}$$

X_i^β represents the nominal composition of the phase β, μ_i^α is the chemical potential of the components in the matrix phase α. Also g^β indicates the Gibbs Free Energy of the precipitates β, *i* stands for the different components in an alloy.

Eq. 2.3 changes the equation for specific volume free energy change to

$$\Delta G_{vol} = -\frac{d_{chem}^{\beta}}{v^{\alpha}} + \Delta G_{vol}^{el} \qquad \textbf{eq. 2.4}$$

where the expression v^α defines the molar volume. [4]

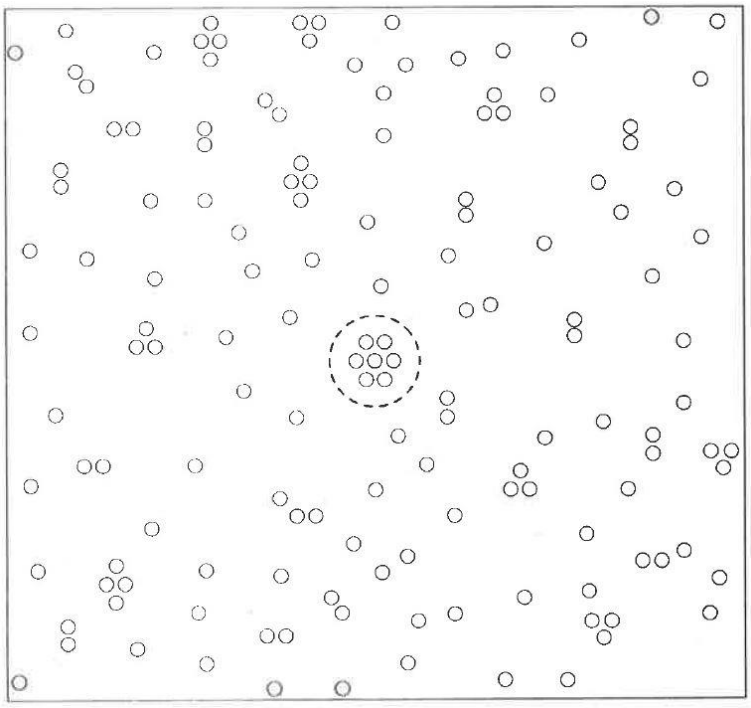

Figure 15: Schematic distribution of monomers, dimers, and so forth, during nucleation, with a critical cluster marked by a dashed cirlce [4]

The graphical interpretation of eq. 2.1, is plotted in Figure 16. Additional the critical radius r^* and the critical nucleation energy G^* are also illustrated. The critical radius r^* indicates the size of a cluster, when it will grow further and will not dissolve again, it gets calculated with

$$r^* = -\frac{2\Delta G_{surf}}{\Delta G_{vol}} = \frac{2\gamma}{\frac{d_{chem}^{\beta}}{v^{\alpha}} + \Delta G_{vol}^{el}}, \qquad \textbf{eq. 2.5}$$

which is the derivative of ΔG_{nucl}, set equal to zero and transformed afterwards. The value of G^* is expressed with

$$G^* = \frac{16\pi}{3}\frac{(\Delta G_{surf})^3}{(\Delta G_{vol})^2} = \frac{16\pi}{3}\frac{\gamma^3}{\left(-\frac{d_{chem}^{\beta}}{\nu^{\alpha}}+\Delta G_{vol}^{el}\right)^2}, \qquad \text{eq. 2.6}$$

which signifies a key quantity for evaluation of the steady-state nucleation rate J_{SS}, which will be discussed in the next section. [4]

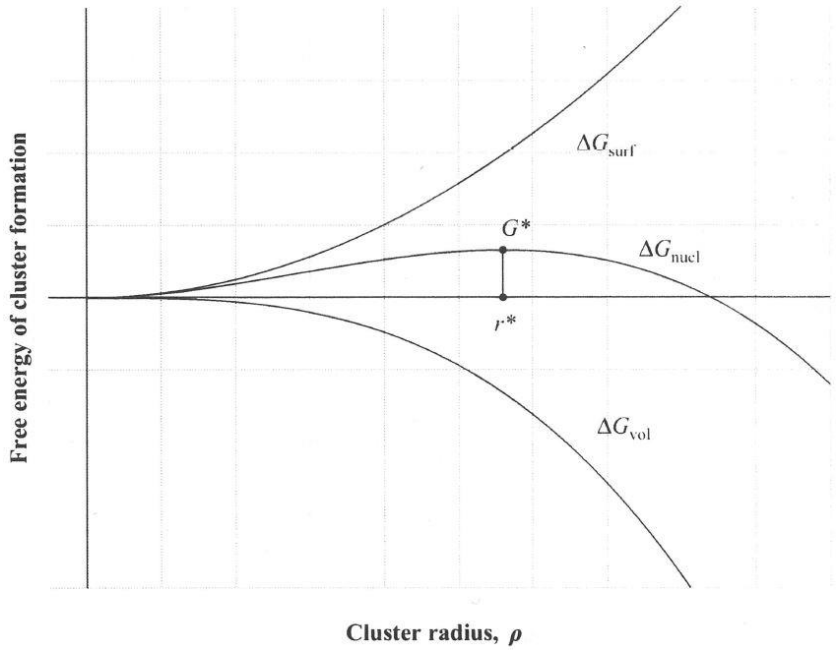

Figure 16: Free energy of cluster formation as a function of the cluster radius [4]

2.2.1.3 Nucleation rate

According to CNT, the steady-state nucleation rate for the formation of a new phase in thermodynamic systems can be expressed by

$$J_{SS} = NZ\beta^* exp\left(-\frac{G^*}{k_B T}\right), \qquad \text{eq. 2.7}$$

where N is the number of potential nucleation sites, Z marks the Zeldovich factor, β^* indicates the atomic attachment rate, G^* stands for the critical nucleation energy as introduced in eq. 2.6, k_B is the Boltzmann constant with a value of 1,380 648 52 · 10^{-23} J/K and T is the absolute temperature. [18]

The Zeldovich factor for the nucleation of a spherical particle is defined with [4]

$$Z = \left[\frac{a^6}{64\pi^2 k_B T} \cdot \frac{(\Delta G_{vol})^4}{(\Delta G_{surf})^3}\right]^{1/2}, \qquad \text{eq. 2.8}$$

which corrects the equilibrium number of critical nuclei to the steady state number of critical nuclei, where a is the interatomic distance [20]. The function of the atomic attachment rate β^* is given with

$$\beta^* = (4\pi)^{\frac{1}{3}}(3v^{\alpha}n^*)^{\frac{2}{3}} D_B \frac{X_B^{\alpha}}{a^4}. \qquad \text{eq. 2.9}$$

D_B is the effective diffusion coefficient, n^* and X_B^{α} are the critical size of a cluster and mole fraction of solute atoms of material B respectively [18].

Eq. 2.7, representing the steady-state nucleation rate, which describes a very general approach, because it is an assumption that at the time t=0 an equilibrium distribution of clusters is present. Practically, it does not meet reality, because the equilibrium distribution of clusters is a function of time, and for different heat treatment processes the temperature varies through time. Therefore, D. Turnbull [21] introduced the following relation between the steady-state and the transient nucleation rate

$$J = J_{SS} exp\left(-\frac{\tau}{t}\right), \qquad \text{eq. 2.10}$$

with t as the time and τ as the induction period or incubation time, which is nowadays used frequently. If J_{ss} is inset from eq. 2.7, the resulting expression for the transient nucleation rate is

$$J = J_{SS} exp\left(-\frac{\tau}{t}\right) = NZ\beta^* exp\left(-\frac{G^*}{k_B T}\right) exp\left(-\frac{\tau}{t}\right). \qquad \text{eq. 2.11}$$

2.2.2 Growth and coarsening

In a continuums-mechanical model of the diffusion-controlled growth of a precipitate, three processes have to be taken in account:

- Diffusion in the particle
- Diffusion in the matrix near to the precipitate
- The interface-movement

Some models introduce simplifications such as ignoring phase boundary energies and assuming equilibrium compositions in particles. The resulting quantity in these growth models is the growth velocity of a precipitate. [22] [23]

2.2.2.1 The Zener model – Binary diffusion-controlled growth

The binary diffusion-controlled growth model was developed by C. M. Zener in 1949, it is a simple solution for the binary moving boundary problem with the assumption of local equilibrium at the interface. The result of his work about the movement of a planar interface between two phases in a two-component system, is the parabolic growth law

$$\rho(t) = \sqrt{\rho_0 + S^2 D t}, \qquad \text{eq. 2.12}$$

where $\rho(t)$ indicates the position of the interface depending on time t, ρ_0 is the initial position, D is the diffusion constant in the matrix and S is the dimensionless supersaturation in the matrix. The dimensionless supersaturation is defined by

$$S = \frac{c_0 - c_{\alpha\beta}}{c_\beta - c_{\alpha\beta}}, \qquad \text{eq. 2.13}$$

where c_0 is the concentration of material B in the matrix in infinite distance from the particle, c_β is the constant concentration inside the precipitate and $c_{\alpha\beta}$ is the equilibrium concentration in the matrix. [22]

2.2.2.2 Precipitate coarsening – The LSW-theory

The LSW-theory is based on the work of F. W. Ostwald, a German chemist, who treated the phenomenon that dispersoid systems change their particle constitution in time [24] [25]. C. W. Wagner [26], I. M. Lifshitz and V. Slyozov [27] independently investigated the so called Ostwald ripening in 1961, hence the name LSW-theory.

The authors developed following expression for the stationary size distribution of the precipitates in a multiparticle system, which is only valid for the equilibrium phase fraction:

$$f(r,t) = \frac{4}{9}\xi^2 \left(\frac{3}{3+\xi}\right)^{\frac{7}{3}} \left(\frac{\frac{3}{2}}{\frac{3}{2}-\xi}\right)^{\frac{11}{3}} exp\left(-\frac{\xi}{\frac{3}{2}-\xi}\right), \qquad \text{eq. 2.14}$$

which converges to a specific shape, shown in Figure 17. In eq. 2.14 ξ denotes the ratio of the radii, which can be read as

$$\xi = \frac{r}{r^*(t)}, \qquad \text{eq. 2.15}$$

where r is the radius of the particle and $r^*(t)$ is the radius of a particle in equilibrium depending on time t. [26]

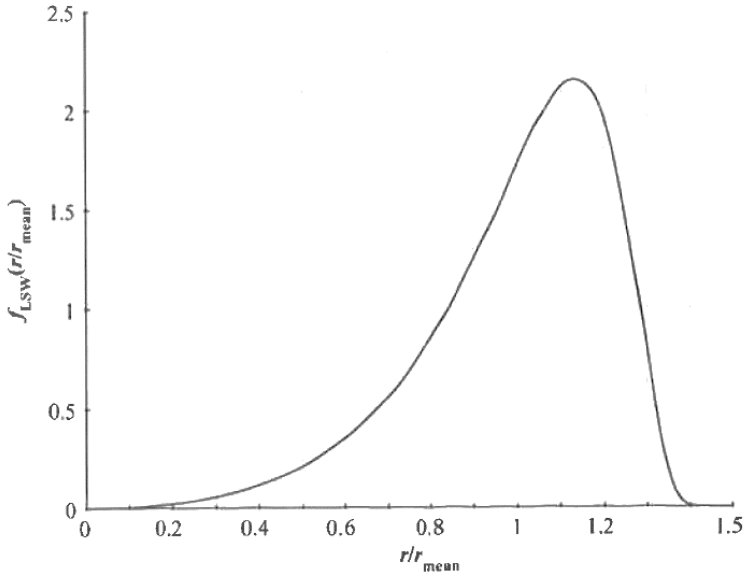

Figure 17: Normalized LSW-function [4]

Lifshitz, Slyozov and Wagner also found a constant coarsening rate, which is expressed by

$$\bar{\rho}^3 - \bar{\rho}_0^3 = Kt \qquad \text{eq. 2.16}$$

with

$$K = \frac{8}{9} \cdot \frac{\gamma D c_e V_m^2}{RT}, \qquad \text{eq. 2.17}$$

where $\bar{\rho}$ denotes the mean radius, $\bar{\rho}_0$ is the initial starting radius, γ is the specific interfacial energy, D is the diffusion coefficient, c_e the solubility of the component in the parent phase, V_m is the molar volume, R, T and t are as usual the ideal gas constant, the absolute temperature and time, respectively. [26] [27]

Furthermore, the LSW-theory was improved by several authors, but this is not treated further, so that the reader is referred to the work of E. Kozeschnik [4].

2.2.2.3 The SFFK-model

The SFFK-model was developed by J. Svoboda, F. D. Fischer, P. Fratzl and E. Kozeschnik [28]–[31] and combines the growth and coarsening mechanisms of particles, including the development of each precipitate composition. This model matches the results from the previous mentioned models, although it is based on a completely different physical concept with parameters, such as the total Gibbs Free Energy and the energy dissipation.

The SFFK-model fits for a multicomponent system with n components and m precipitates with dissimilar size and phase type in a matrix. The Gibbs Free Energy can be calculated with

$$G = \sum_{i=1}^{n} N_{0i}\mu_{0i} + \sum_{k=1}^{m} \frac{4\pi\rho_k^3}{3}(\lambda_k + \sum_{i=1}^{n} c_{ki}\mu_{ki}) + \sum_{k=1}^{m} 4\pi\rho_k^2\gamma_k \qquad \text{eq. 2.18}$$

where N_{0i} is the number of moles of a component *i* in the parent phase, μ_{0i} is the appropriate chemical potential, λ_k describes the elastic energy due to volumetric misfit, ρ_k is the radius of a particle *k*, c_{ki} is the concentration of component *i* in the precipitate *k*, μ_{ki} is the appropriate chemical potential and γ_k is the interfacial energy of a precipitate *k*. The first term of eq. 2.18 represents the Gibbs Free Energy of the matrix, the second term describes the bulk free energies of all precipitates and the third part is the energy contribution of the precipitate matrix interface.

2.2.3 The GBB-model – calculation of interfacial energies

The GBB-model is based on the Nearest-Neighbor Broken-Bond (NNBB) model, introduced by R. Becker in 1938 [32], which is a simple and powerful framework for the calculation of interfacial energies. The NNBB-model describes the interfacial energy as the difference in total energy, if two separated blocks of homogeneous phases, X_i^M and X_i^P, are cut in half and the dissimilar pieces are reassembled, see Figure 18. This concludes in the following relation for the interfacial energy:

$$\gamma = \frac{n_s z_s}{N_A z_L} \cdot \Delta H_{sol} \qquad \text{eq. 2.19}$$

where n_S marks the number of atoms per unit area of interface, z_S is the number of broken bonds across the interface per interface atom, N_A is the Avogadro's number, z_L is the number of nearest-neighbor positions and ΔH_{sol} denotes the enthalpy of the solution.

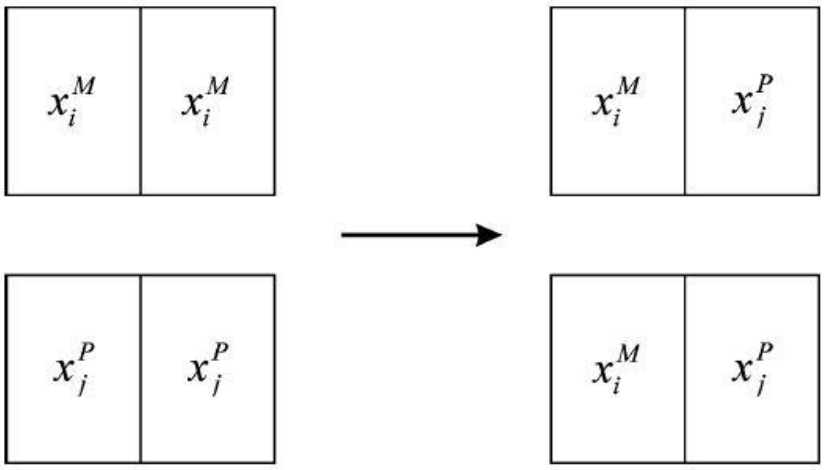

Figure 18: Calculation scheme of the interfacial energy [33]

B. Sonderegger and E. Kozeschnik [33] found in 2009 the potential for improvements of the NNBB-model and developed the Generalized Broken-Bond (GBB) model, which also takes the n-nearest

neighbor interaction across the interface in account. The result was a more general expression for the interfacial energy:

$$\gamma = \frac{n_s z_{s,eff}}{N_A z_{L,eff}} \cdot \Delta H_{sol} \qquad \text{eq. 2.20}$$

where $z_{S,eff}$ is the effective number of broken bonds across the interface and $z_{L,eff}$ is the effective number of nearest neighbor positions, dependent on a weighting function $f(r_k/r_1)$ with *k* as the index of the coordination shell and *1* representing the first-nearest neighbor shell. In addition, they proved concept is also valid for multicomponent systems.

2.3 MatCalc – The MATerials CALculator

The development of the program MatCalc started with the PhD thesis of E. Kozeschnik at the Graz University of Technology, Austria in 1993. In the following years, the software package was improved and in 2004, the fundamental relations of the MatCalc growth model were published [29] [34]. The software is based on three modules, where certain calculations can be executed [4]:

1. Equilibrium thermodynamics
   a. Phase diagrams and phase fraction diagrams
   b. Constrained equilibrium and non-equilibrium thermodynamics
   c. Scheil-Gulliver type simulations
   d. T_0-temperature calculations

2. Precipitation kinetics
   a. Nucleation and growth kinetics of individual precipitates
   b. Evolution of precipitate distributions
   c. Precipitation sequences with metastable phases
   d. Thermo-mechanical treatments of alloys
   e. Isothermal and continuous Time-Temperature-Precipitation diagrams
   f. Evolution of quenched-in vacancies
   g. Precipitation strengthening
   h. Evolution of dislocation density and grain size during deformation
   i. Grain growth in the presence of precipitates

3. Microstructure evolution
   a. Thermal and multi-component diffusion field simulation
   b. Simultaneous precipitation and long-range diffusion
   c. Moving phase boundaries

The first module, equilibrium thermodynamics, acts as assistant module for the other two. It contributes the necessary thermodynamic quantities and is used by the precipitation kinetics and microstructure evolution modules. [4]

To serve all this functions, MatCalc works with different models and theories, for the nucleation it is based on multicomponent CNT (see chapter 2.2.1.3), for the calculation of interfacial energies it uses the GBB-model (see chapter 2.2.3), for the evolution of precipitates the SFFK-model (see chapter 2.2.2.3) and as kinetic model, the Numerical Kampmann-Wagner (NKW) Model was chosen as well as the thermodynamics and mobility origins from the CALPHAD-type database. [4]

For a better understanding, how MatCalc is operating, here is a short description of the Kampmann-Wagner methodology [35], which is also graphically shown in Figure 19:

- Considering a system with unit volume and divide the time into discrete intervals Δt
- Evaluation of the nucleation rate (eq. 2.11) for the actual time period.
    - If $J > 0$:
        - Creation of $N_{m+1} = J(t)\Delta t$ precipitates and collection of all new N_{m+1} precipitates in a precipitate class with identical radius ρ_{m+1} and identical composition. (m being the number of existing precipitate classes in the class array)
        - Assigning a radius ρ_{m+1} to the precipitate class, which is slightly larger than the critical nucleation radius r^* (eq. 2.5)
- Evolving the radius ρ_k of all existing precipitate classes according to $\Delta\rho_k = \dot{\rho}\Delta t$, with $k = 1, \dots, m$.
- If the radius ρ_k of a precipitate class drops below a certain limit, the removal of the precipitate class from the array takes place and m is decreased by 1.
- If a new class of precipitates has been nucleated, m is increased by 1.
- Repeating these steps until the finish time is reached.

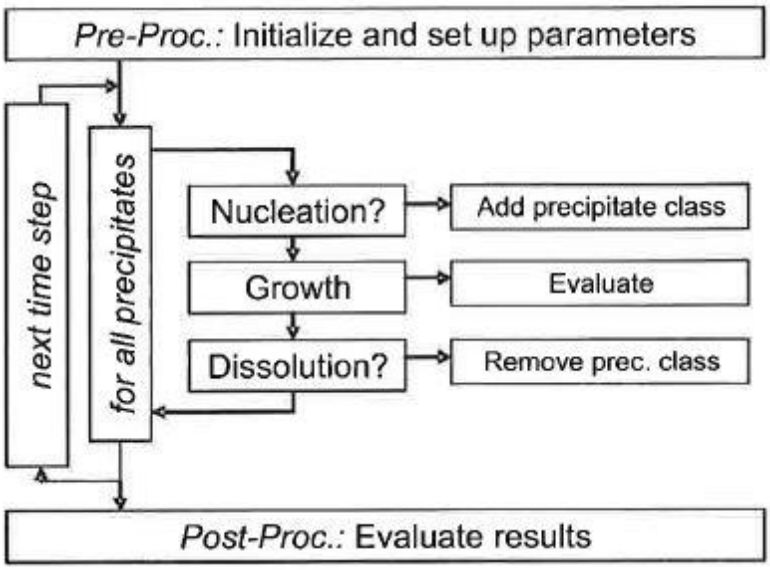

Figure 19: Typical scheme for numerical integration of the evolution equations according to the numerical Kampmann-Wagner model [4]

For the sake of completeness, also the CALPHAD approach is shortly described in this section. CALPHAD is the abbreviation for "CALculation of PHAse Diagrams" and has been developed in the early 1970s. It

provides the basis for practically all advanced software for computational thermodynamics that is nowadays available. It is a framework for the numerical evaluation of multicomponent multiphase phase equilibria. [4]

"Real" thermodynamic systems include complex chemical interactions, which cannot be described through an ideal or a regular solution, but an ideal solution model can be taken as a reference state and expresses the properties of the real system in terms of excess quantities. Basically, the CALPHAD approach uses Redlich-Kister polynomial series to describe excess Gibbs energies, which are defined as

$$^{ex}G_m = \sum_{i \neq j} {}^{k}L_{ij} \cdot X_i X_j \left(X_i - X_j\right)^k, \qquad \textbf{eq. 2.21}$$

where the indices *i* and *j* describe two components, ${}^{k}L_{ij}$ is called the interaction parameter and describes the intensity of the excess interaction between the components. The exponent *k* is an integer and marks the order of the Redlich-Kister polynomial, and X_i and X_j are the prevailing mole fractions of the components. [4]

3. Numerical Simulations

This chapter gives an overview about the computer system properties, the software versions and the used thermodynamic and diffusion databases. Furthermore, it is described how the main parameters, like compositions and heat treatments, for the calculations have been set up and executed.

3.1 Computer, software and databases

All calculations were performed with the same computer-system and software, with the most important properties are listed in Table 1.

Table 1: Computer, Software and database versions

Processor:	Intel Core i5-750 CPU with 2,67 GHz and 8M Cache
Installed main memory (RAM):	8,00 GB
Operating system:	Microsoft Windows 7 Enterprise with Service Pack 1
System type:	64 Bit Operating System
MatCalc version:	Version 5.60
Thermodynamic database:	mc_al_v2.001.tdb
Diffusion database:	mc_al_v2.001.ddb

3.2 Equilibrium phase diagram calculation

For the calculations of the liquid phase boundaries, the solid Al-matrix phase and Al_3Sc phase boundaries in the equilibrium phase diagram, a composition of 0,05 wt.% Sc and 99,95 wt.% Al was chosen randomly. The calculation was performed in the field of 10^{-5} – 30 wt.% Sc with a step interval of 0,005 wt.%, and the temperature ranged between -273 °C to 6000 °C, where MatCalc is fundamentally able to calculate the different Gibbs Free Energies. The calculation comprised the Al-matrix phase FCC_A1, the liquid phase and the intermetallic phase Al_3Sc. The calculation is in more detail described in section 4.1.1. Later the positions of the boundaries were compared with the ones from the literature.

3.3 Precipitation kinetics calculation

For the precipitation simulations, several heat treatments of different Al-Sc alloys were extracted from the literature. Table 2 lists the different heat treatments and compositions with their corresponding sources. Additionally, the shorthand symbols are listed for the treatment in this thesis. Afterwards, the resulting precipitate radii, precipitate numbers, phase fractions and nucleation rates were evaluated (see chapter 4.2).

Owing to the fact that in most papers neither heating nor cooling rates are recorded, the simulations were performed with following assumptions:

- The heating duration was for all heat-ups 300 s
- The cooling duration was for all quenchings 10 s

Table 2: Heat treatments and compositions for the precipitation kinetic simulations

Reference	Shorthand Symbol	Heat Treatment	Composition
Marquis E.A. [36]	Marquis_1	648 °C for 24 h + Quenching + 300 °C for 6 h + Quenching	Al-0,3 wt.% Sc
	Marquis_2	648 °C for 24 h + Quenching + 350 °C for 24 h + Quenching	Al-0,3 wt.% Sc
	Marquis_3	648 °C for 24 h + Quenching + 400 °C for 1 h + Quenching	Al-0,3 wt.% Sc
	Marquis_4	648 °C for 24 h + Quenching + 400 °C for 120 h + Quenching	Al-0,3 wt.% Sc
	Marquis_5	648 °C for 24 h + Quenching + 300 °C for 72 h + Quenching	Al-0,1 wt.% Sc
	Marquis_6	648 °C for 24 h + Quenching + 300 °C for 72 h + Quenching	Al-0,2 wt.% Sc
	Marquis_7	648 °C for 24 h + Quenching + 300 °C for 72 h + Quenching	Al-0,3 wt.% Sc
	Marquis_8	648 °C for 24 h + Quenching + 450 °C for 72 h + Quenching	Al-0,3 wt.% Sc
	Marquis_9	648 °C for 24 h + Quenching + 300 °C for 120 h + Quenching	Al-0,3 wt.% Sc
	Marquis_10	648 °C for 24 h + Quenching + 300 °C for 350 h + Quenching	Al-0,3 wt.% Sc
Berezina et al. [37]	Berezina	isothermal at 300 °C for 350 h	Al-0,3 wt.% Sc
Sano et al. [13]	Sano	isothermal at 300 °C for $6x10^5$ s	Al-0,25 wt.% Sc
Miura et al. [13]	Miura	isothermal at 350 °C for 10^6 s	Al-0,23 wt.% Sc
Novotny G. [38]	Novotny_1	642 °C for 2 h + Quenching + 350 °C for 72 h + Quenching	Al-0,3 wt.% Sc
	Novotny_2	642 °C for 2 h + Quenching + 350 °C for 6 months + Quenching	Al-0,2 wt.% Sc
Iwamura S. [39]	Iwamura_1	640 °C for 2 h + Quenching + 400 °C for 10^6 s + Quenching	Al-0,2 wt.% Sc
	Iwamura_2	640 °C for 2 h + Quenching + 430 °C for 10^6 s + Quenching	Al-0,2 wt.% Sc
	Iwamura_3	640 °C for 2 h + Quenching + 460 °C for 10^6 s + Quenching	Al-0,2 wt.% Sc
	Iwamura_4	640 °C for 2 h + Quenching + 490°C for 10^6 s+ Quenching	Al-0,2 wt.% Sc
Robson J.D. [40]	Robson_1	640 °C for 72 h + Quenching + 400 °C for 1 h + Quenching	Al-0,25 wt.% Sc
	Robson_2	640 °C for 72 h + Quenching + 450 °C for 1 h + Quenching	Al-0,25 wt.% Sc
	Robson_3	640 °C for 72 h + Quenching + 500 °C for 1 h + Quenching	Al-0,25 wt.% Sc
	Robson_4	640 °C for 72 h + Quenching + 550 °C for 1 h + Quenching	Al-0,25 wt.% Sc
	Robson_5	isothermal 343 °C for 1 h	Al-0,11 at.% Sc
Clouet E. [41]	Clouet_1	isothermal at 300 °C for 10^6 s	Al-0,18 at.% Sc
	Clouet_2	isothermal at 350 °C for 10^6 s	Al-0,18 at.% Sc
	Clouet_3	isothermal at 300 °C for 10^6 s	Al-0,18 at.% Sc
Royset [13]	Royset_1	600 °C for 1 h + Quenching to 230 °C and holding 170 h + Quenching	Al-0,2 wt.% Sc
	Royset_2	600 °C for 1 h + Quenching to 270 °C and holding 170 h + Quenching	Al-0,2 wt.% Sc
	Royset_3	600 °C for 1 h + Quenching to 330 °C and holding 170 h + Quenching	Al-0,2 wt.% Sc
	Royset_4	600 °C for 1 h + Quenching to 370 °C and holding 170 h + Quenching	Al-0,2 wt.% Sc

4. Results

The results of the different calculations, with and without changed parameters, are presented in this chapter. Additionally, the deviations between the literature and the calculated quantities are discussed.

4.1 Equilibrium phase diagrams

The calculations were performed as described in section 3.2 and a closer look on the results is given here.

4.1.1 Standard calculations

The resulting equilibrium phase diagram based on the standard database is shown in Figure 20, the relevant script for the calculation can be found in appendix A). The calculation was performed in the field of 10^{-5} – 30 wt.% Sc with a step interval of 0,005 wt.% and the temperature range was between -273 °C to 6000 °C.

No computational errors occurred with the calculation of the liquid phase boundary and the solid Al-matrix phase, but with the calculation of the Al_3Sc-phase. Normally, the software calculates the boundary of a phase constantly in one simulation, but in this case it did not. Therefore, the Al_3Sc-phase boundary had to be split in to two calculations.

The same parameters were used in the calculations of the Al_3Sc-phase as well as other phase-boundaries, but the program decreased the increment at a concentration of approximately 0,3 wt.% Sc. It stopped working after reaching the maximum number of iterations at a concentration of approximately 0,31 wt.% Sc. For detecting the failure of the concentration, the composition was changed from 0,05 wt.% Sc to 1,0 wt.% Sc. The calculation started again with these parameters and reached the point of error from the other direction by decreasing the concentration, instead of increasing. The same error appeared at a concentration of 0,24 wt.% Sc. For a better understanding, of this calculation problem, a detailed view of the eutectic and the surrounding boundaries were plotted in Figure 21.

The green and violet lines in Figure 21 represent the Al_3Sc boundaries, whereas the red and blue lines define the boundaries of the solid Al-matrix and liquid phase. At the first glance, it can be noticed that the boundaries of the primary and secondary Al_3Sc phases are overlapping in direction of the Sc-content, which is not physically possible and therefore can be treated as the cause of the error. The second difference is the not well positioned and non-aligned area of the liquid phase and solid Al-matrix, as resulting area of the red and blue lines.

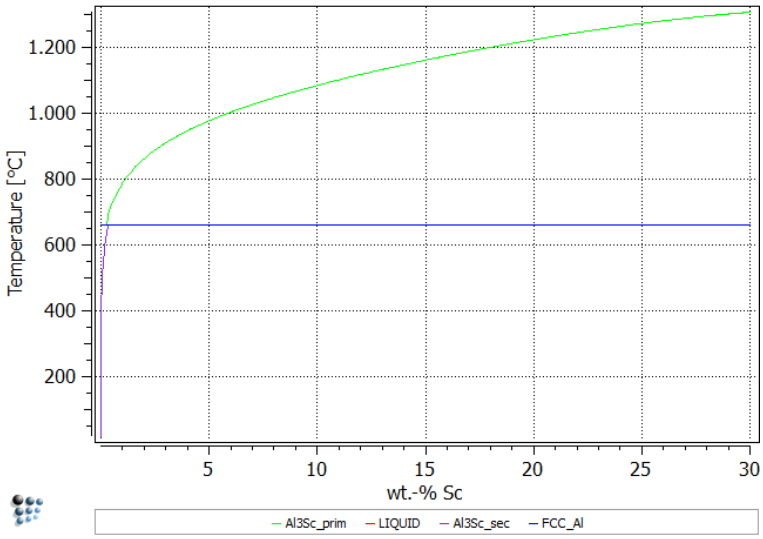

Figure 20: Equilibrium phase diagram based on the original database

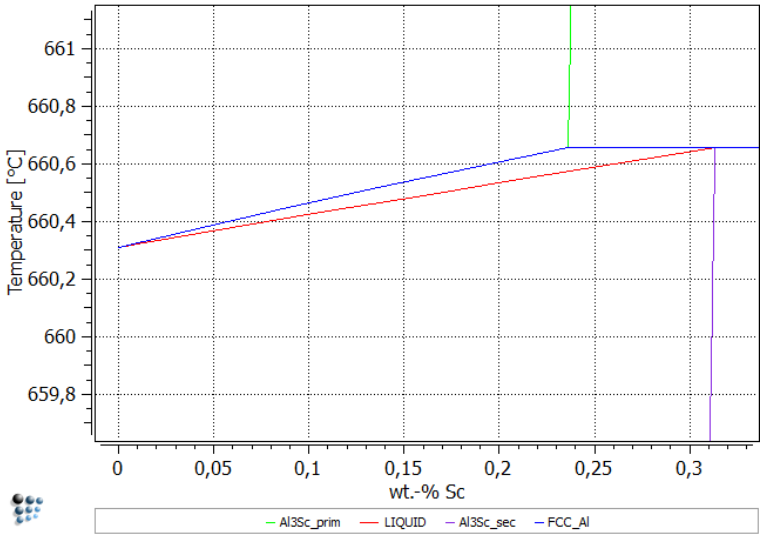

Figure 21: Detailed view of the equilibrium phase diagram based on the original database

4.1.2 Discussion

The reference values for the calculations of the equilibrium phase diagram were gathered from Figure 2 and Figure 4 [9]. These values were added to the equilibrium phase diagram and are illustrated in Figure 22. It is evident that the boundary of the Al_3Sc-phase (green line) in the higher Sc-content region is overestimated by the thermodynamic database. A detailed view of the Sc-low region in Figure 23 shows that the Al_3Sc-phase boundaries has to be shifted to the right. As mentioned before, there is no clear eutectic point because of the overlapping of the Al_3Sc-phase boundaries, and the primary boundary has to be stronger shifted to the right. In the before mentioned section, in this field the error occurred. The reason for this is the software could not find the next point of the boundary, because the increment cannot switch in another direction during calculation, except if one of the calculation constraints (in this case: 10^{-5} and 30 wt.% Sc) is reached.

According to Royset & Ryum [9], the eutectic should be at a temperature of 655 °C and a Sc-concentration of about 0,55 wt.%, as it is visible in Table 3. There is an absolute deviation of 80,14 °C between measured and calculated solubility temperature of Al_3Sc and the expected eutectic could range between 0,24 – 0,3 wt.% Sc.

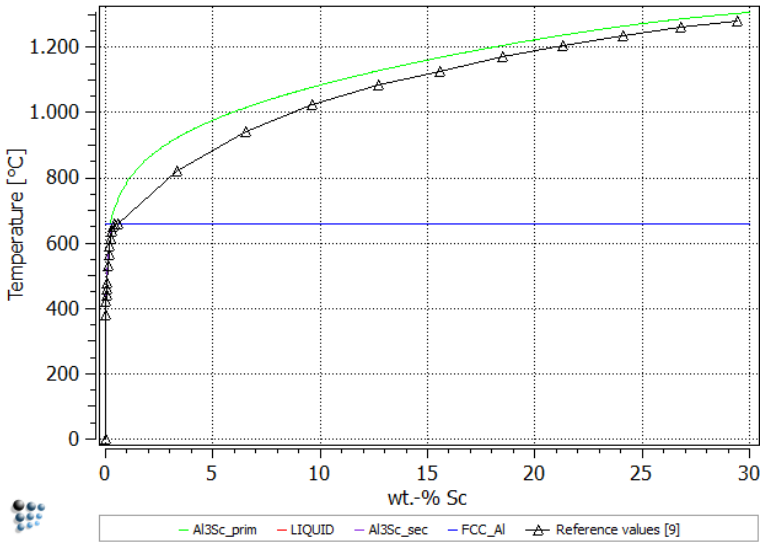

Figure 22: Comparison of the standard-calculated equilibrium phase diagram with the reference values

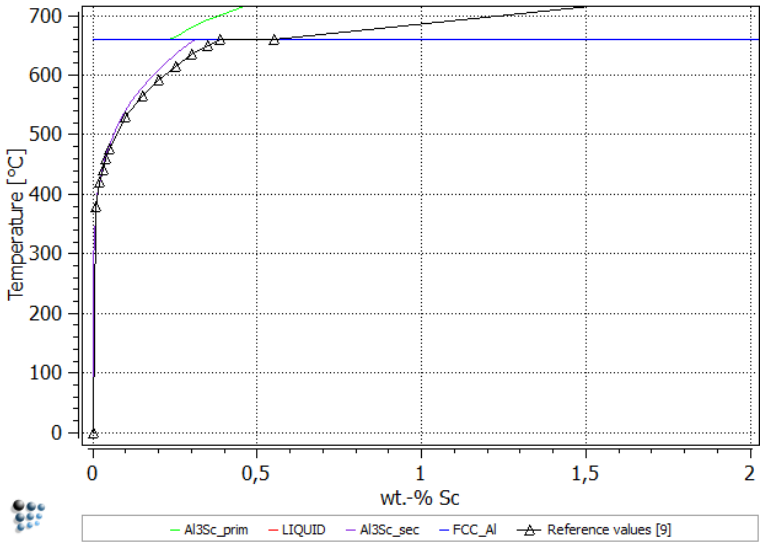

Figure 23: Detailed view of the comparison of the standard-calculated equilibrium phase diagram with the reference values

Table 3: Results and deviations of the standard equilibrium phase diagram calculation

Sc-concentration		Solubility temperature of Al_3Sc [°C]		Deviations	
wt.%	at.%	Literature [9]	Calculated	abs. [°C]	%
0,01	0,006	380	376,98	-3,02	-0,46
0,02	0,012	420	418,84	-1,16	-0,17
0,03	0,018	442	445,97	3,97	0,56
0,04	0,02	460	466,58	6,58	0,90
0,05	0,03	477	483,43	6,43	0,86
0,10	0,06	530	541,29	11,29	1,41
0,15	0,09	566	576,7	10,7	1,28
0,20	0,12	592	609,43	17,43	2,01
0,25	0,15	615	634,11	19,11	2,15
0,30	0,18	635	655,44	20,44	2,25
0,35	0,21	650	692,26	42,26	4,58
0,39	0,23	660	700,24	40,24	4,31
0,55	0,36	659	739,14	80,14	8,60
3,30	2	820	921	101	9,24
6,50	4	940	1014	74	6,10
9,60	6	1025	1077	52	4,01
12,70	8	1085	1128	43	3,17
15,60	10	1120	1169	49	3,52
18,50	12	1170	1205	35	2,43
21,30	14	1205	1237	32	2,16
24,10	16	1235	1264	29	1,92
26,80	18	1260	1286	26	1,70
29,40	20	1280	1303	23	1,48

4.1.3 Optimized calculations

This section is divided into two parts, the first part treats calculations which have been made by the author, but are not permitted according to CALPHAD and E. Povoden-Karadeniz, an Assoc.-Prof. at the Institute of Materials Science and Technology in Vienna [42] [43]. The second part describes the approach which is allowed.

For moving the equilibrium phase diagram to the right position and debug the calculation in the range between 0,24 – 0,31 wt.% Sc, it was necessary to change several parameters in MatCalc. All parameters, which were changed for different approaches for the optimization of the equilibrium phase diagram are listed in Table 4.

Table 4: Changed database parameters due to the optimization of the equilibrium phase diagram

Parameter	Change permitted	Description
G(LIQUID,AL,SC;0)	YES	Liquid interaction-parameter, which represent the energies of mixture of an Al-melt with a Sc-melt
G(LIQUID,AL,SC;1)	YES	a/m
G(LIQUID,AL,SC;2)	YES	a/m
G(FCC_A1,AL,SC:VA;0)	YES	Gibbs Free Energy of the Al-matrix
G(AL3SC,AL:SC;0)	YES	Gibbs Free Energy of an Al_3Sc-particle
SE(Al3SC)	NO	Offset parameter for the output, does not influence calculation
G(LIQUID,SC;0)	NO	Gibbs Free Energy of liquid Sc
G(Al3SC,AL:SC;0)	YES	Gibbs Free Energy of an Al_3Sc-precipitate
G(FCC_Al,SC:VA;0)	NO	Gibbs Free Energy of Sc in Al-matrix

4.1.3.1 Prohibited approaches

The modeling of the equilibrium phase diagram started randomly with the variation of different parameters. After some time, several attempts with better convergence than the original approach were found. The fact that the following calculations are not compatible to restrictions by the CALPHAD-community [42], should not be forgotten, but these approaches should give a hint for further investigations.

Approach 1

In this approach the parameters SE(Al3SC) and G(LIQUID,SC;0) were changed and the values are shown in Table 5, with the graphical results are plotted in Figure 24 and detailed in Figure 25. These changes led to a good positioning of the eutectic and an accurate convergence with the reference values till 5 wt.% Sc. The parameter SE(Al3SC) does only change the output in the graphical user interface and does not affect the calculation which is therefore no database-value, and G(LIQUID,SC;0) is not allowed to be changed according to CALPHAD. [42]

Table 5: Changed parameter values of approach 1

Parameter	Original value	Modified value
SE(Al3SC)	298,16 **0,0**; 6000 N	298,16 **400,0**; 6000 N
G(LIQUID,SC;0)	273 +1*GSCLIQ#; 3200 N	273 **-5070**+1*GSCLIQ#; 3200 N

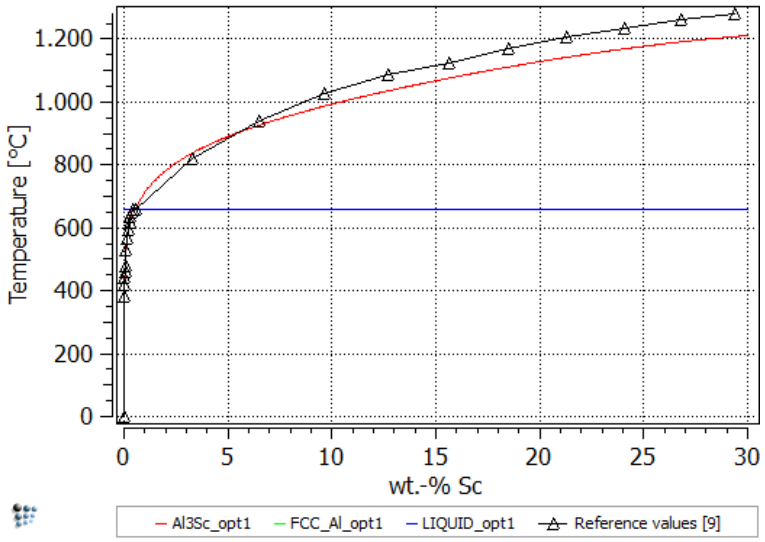

Figure 24: Equilibrium phase diagram according to approach 1

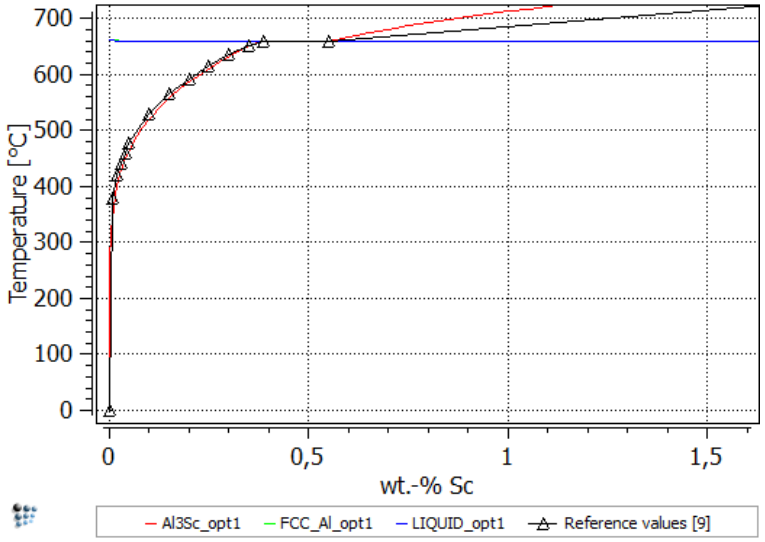

Figure 25: Detailed view of the equilibrium phase diagram according to approach 1

Approach 2

The second approach shows a better convergence above the concentration of 12 wt.% Sc, but below 12 wt.% Sc the similarity were reduced and the eutectic shifted, as discernable in Figure 26 and Figure 27, with a detailed view of the low Sc-area. This approach contains the changes of approach 1 with the additional modification of G(Al3Sc,Al:Sc;0), listed in Table 6.

Table 6: Changed parameter values of approach 2

Parameter	Original value	Modified value
SE(Al3SC)	298,16 **0,0**; 6000 N	298,16 **400,0**; 6000 N
G(LIQUID,SC;0)	273 +1*GSCLIQ#; 3200 N	273 **-5070**+1*GSCLIQ#; 3200 N
G(Al3SC,AL:SC;0)	273 -168000+14,75*T +3*GHSERAL#+**1***GHSERSC#; 6000 N	273 -168000+14,75*T +3*GHSERAL#+**1,05***GHSERSC#; 6000 N

Parameter G(Al3SC,Al:SC;0) is allowed to be changed, but that should happen in a stoichiometric correct way, because it describes the Gibbs Free Energy of the Al_3Sc-precipitates. Hence, the value of 1,05 is not allowed to be used. [42]

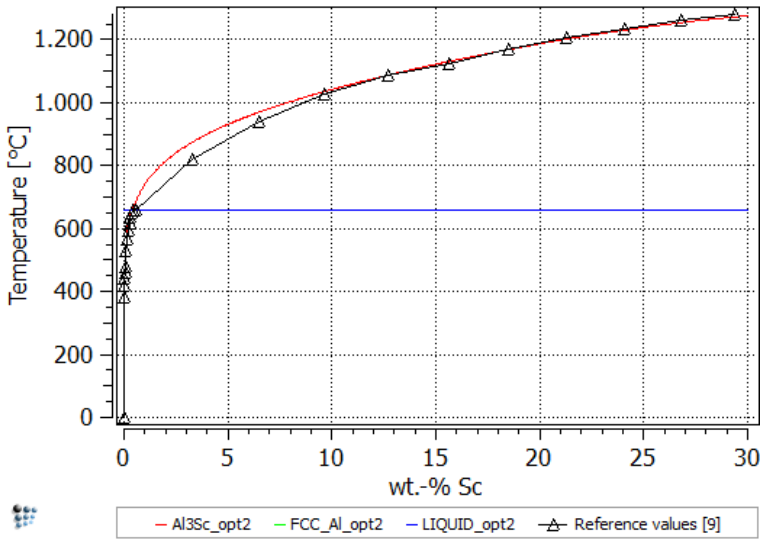

Figure 26: Equilibrium phase diagram according to approach 2

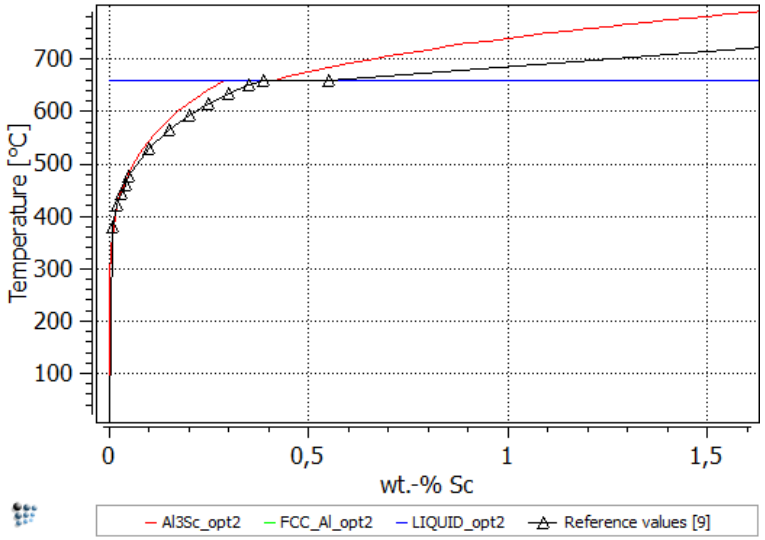

Figure 27: Detailed view of the equilibrium phase diagram according to approach 2

Approach 3

For this approach, additional to approach 2, the parameter SE(Al3Sc) was increased as listed in Table 7. Figure 28 shows that this modification led to a better convergence in the lower Sc-area, but not as good as in approach 1. In Figure 29 the worse correspondence in the higher Sc-area, compared to approach 2, is shown. The restrictions of the parameters are still the same as in approach 2.

Table 7: Changed parameter values of approach 3

Parameter	Original value	Modified value
SE(Al3SC)	298,16 **0,0**; 6000 N	298,16 **800,0**; 6000 N
G(LIQUID,SC;0)	273 +1*GSCLIQ#; 3200 N	273 **-5070**+1*GSCLIQ#; 3200 N
G(Al3Sc,AL:SC;0)	273 -168000+14,75*T+3*GHSERAL# +**1***GHSERSC#; 6000 N	273 -168000+14,75*T+3*GHSERAL#+ **1,05***GHSERSC#; 6000 N

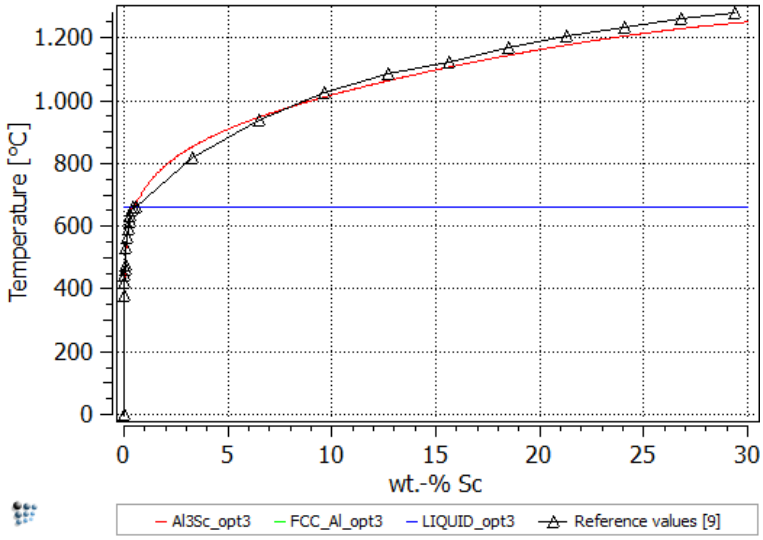

Figure 28: Equilibrium phase diagram according to approach 3

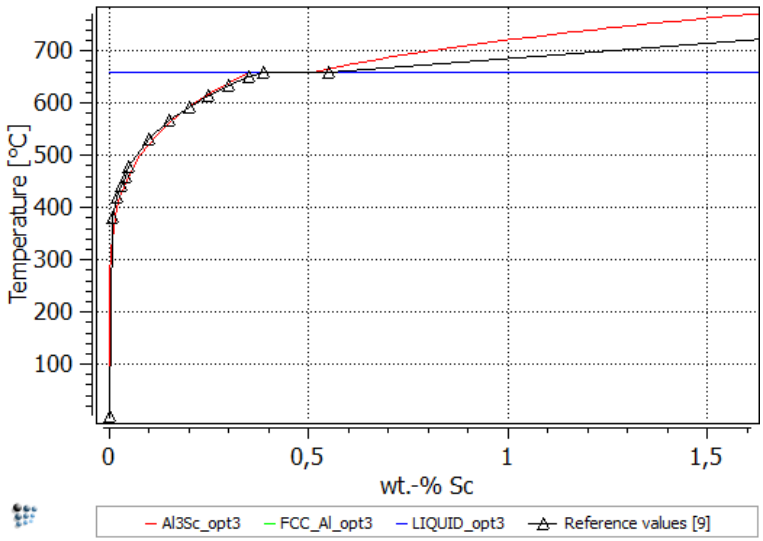

Figure 29: Detailed view of the equilibrium phase diagram according to approach 3

Approach 4

In this approach, five changes were performed, which led to a highly accurate Sc-low area and an inaccurate Sc-high area, as shown in Figure 30 and Figure 31. However, the different changes made the calculation unnecessary complicated. As shown in Table 8, additional the parameter

G(FCC_Al,Sc:Va;0) was changed, whereby this parameter is also restricted to be changed according to CALPHAD.

Table 8: Changed parameter values of approach 4

Parameter	Original value	Modified value
SE(Al3SC)	298,16 **0,0**; 6000 N	298,16 **400,0**; 6000 N
G(LIQUID,SC;0)	273 +**1***GSCLIQ#; 3200 N	273 **-5070**+**1,06***GSCLIQ#; 3200 N
G(AL3SC,AL:SC;0)	273 -168000+14,75*T+3*GHSERAL# +**1***GHSERSC#; 6000 N	273 -168000+14,75*T+3*GHSERAL# +**1,05***GHSERSC#; 6000 N
G(FCC_Al,SC:VA;0)	273 +**1***GSCFCC#; 3600 N	273 +**1,05***GSCFCC#; 3600 N

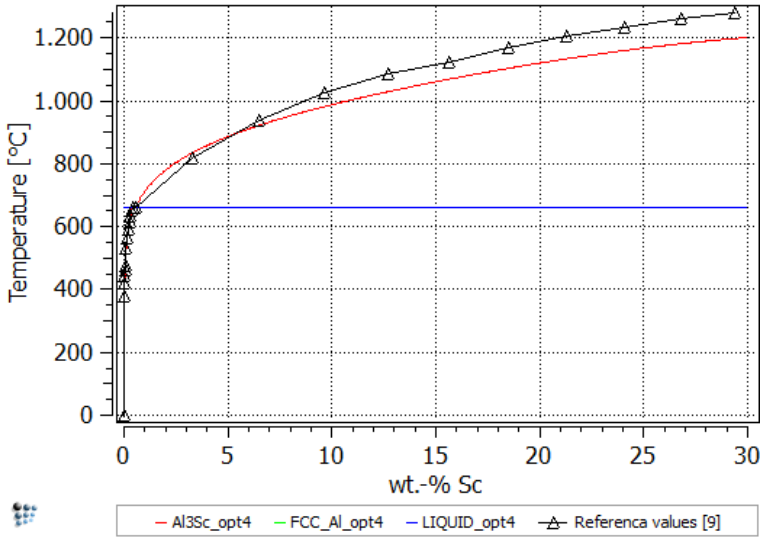

Figure 30: Equilibrium phase diagram according to approach 4

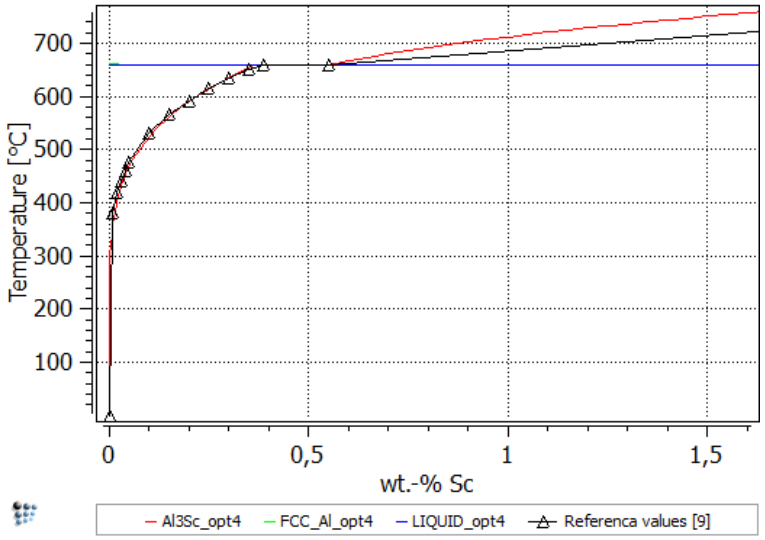

Figure 31: Detailed view of the equilibrium phase diagram according to approach 4

The scripts of the calculations can be seen in the appendix in the sections B) to E) as well as the corresponding results with the calculated deviations in the appendix under section DD).

4.1.3.2 Permitted approach

The last approach of the equilibrium phase diagram was performed with changes of parameters, which were suggested by E. Povoden-Karadeniz [42]. Changed were the liquid-interaction parameters G(LIQUID,AL,SC;0) and G(LIQUID,AL,SC;1), as well as G(FCC_A1,AL,SC:VA;0), which indicates the Gibbs Free Energy of the Al parent-phase. The differences between the original and new values have a manageable size and are indexed in Table 9.

Table 9: Changed parameter values of the final approach

Parameter	Original value	Modified value
G(LIQUID,AL,SC;0)	273 **-155000**+10*T; 6000 N	273 **-163000**+10*T; 6000 N
G(LIQUID,AL,SC;1)	273 **+20000**; 6000 N	273 **+21300**; 6000 N
G(FCC_A1,AL,SC:VA;0)	273 **-110876**; 6000 N	273 **-112376**; 6000 N

The variation of the parameters led to a permitted approach, which are conform with the reference values from the literature.

The parameter G(LIQUID,AL,SC;0) was decreased by 8000 J/mol, which led do a downward movement of the eutectic point to a lower temperature and shifted the primary Al_3Sc area to the right. This indicates an increase of the solubility of Sc in liquid Al.

The parameter G(LIQUID,AL,SC;1) placed the eutectic point on an accurate horizontal position, by increasing its value from 20000 J/mol to 21300 J/mol.

The last parameter G(FCC_A1,AL,SC:VA;0) was adjusted with an increase of 1500 J/mol and shifted the secondary Al_3Sc-region to the right, which performed an abatement of the Sc-solubility in the solid Al-matrix.

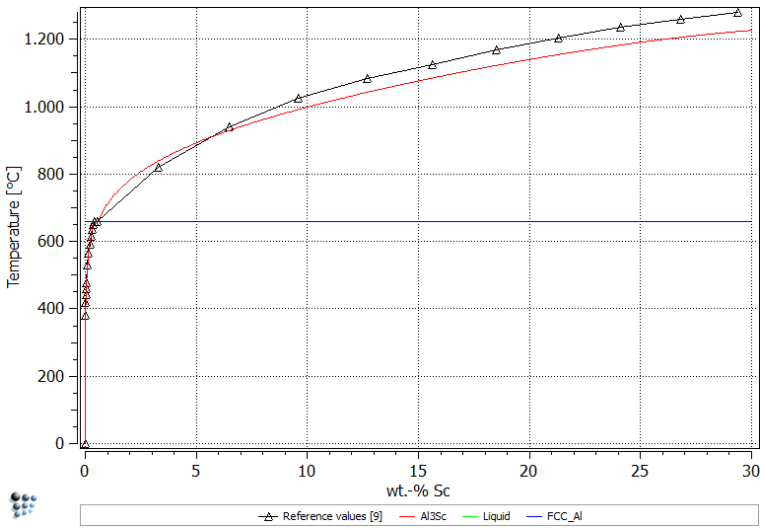

Figure 32: Equilibrium phase diagram according to the final approach

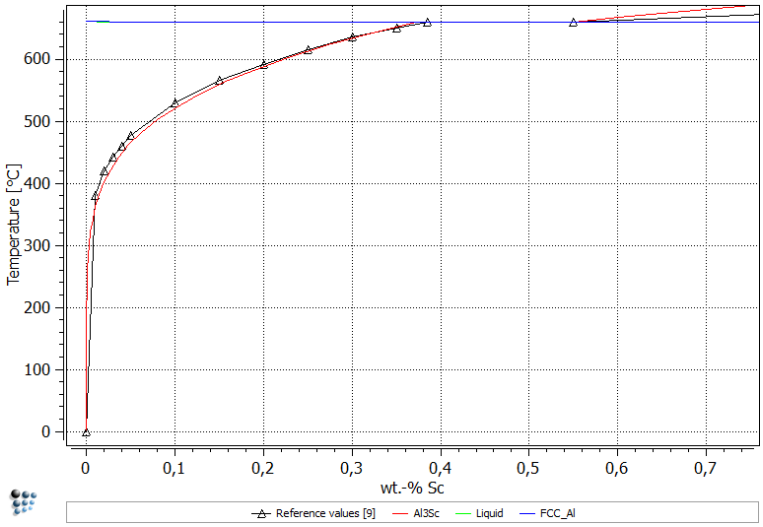

Figure 33: Detailed view of the equilibrium phase diagram according to the permitted approach

The results of the optimized calculations of the permitted approach are graphically presented in Figure 32 and Figure 33, the entire equilibrium phase diagram and the detailed view from it. It is evident that this approach conforms to the reference in the aggregate equilibrium phase diagram. This is confirmed in Table 10, where the calculated points are compared to the literature values and the deviations are determined.

The maximum deviation can be found in the last row at a concentration of 29,4 wt.% Sc with -3,64 %, all other differences are smaller. In the most important region for further kinetic simulations, between 0,1 – 3,3 wt.% Sc, the variance is not larger than 1,79 % and at most points not bigger than 1 %. It is also worth mentioning that, at the eutectic, the deviation is only 0,07 %, which is 0,61 °C.

The script of these calculations can also be found in the appendix in section F) and for a direct comparison with the other approaches, the values from Table 10 are again mentioned in part DD).

Table 10: Results and deviations of the optimized equilibrium phase diagram calculation

Sc-concentration		Solubility temperature of Al_3Sc [°C]		Deviation	
wt.%	at.%	Reference	Calculated	abs. [°C]	%
0,01	0,006	380	362,26	-17,74	-2,72
0,02	0,012	420	402,26	-17,74	-2,56
0,03	0,018	442	428,13	-13,87	-1,94
0,04	0,02	460	448,28	-11,72	-1,60
0,05	0,03	477	464,95	-12,05	-1,61
0,10	0,06	530	522,26	-7,74	-0,96
0,15	0,09	566	559,01	-6,99	-0,83
0,20	0,12	592	587,98	-4,02	-0,46
0,25	0,15	615	612,06	-2,94	-0,33
0,30	0,18	635	632,94	-2,06	-0,23
0,35	0,21	650	651,53	1,53	0,17
0,39	0,23	660	659,61	-0,39	-0,04
0,55	0,36	659	659,61	0,61	0,07
3,30	2	820	839,6	19,6	1,79
6,50	4	940	929,91	-10,09	-0,83
9,60	6	1025	991,91	-33,09	-2,55
12,70	8	1085	1043,06	-41,94	-3,09
15,60	10	1120	1084,97	-35,03	-2,51
18,50	12	1170	1122,46	-47,54	-3,29
21,30	14	1205	1154,75	-50,25	-3,40
24,10	16	1235	1183,01	-51,99	-3,45
26,80	18	1260	1205,99	-54,01	-3,52
29,40	20	1280	1223,54	-56,46	-3,64

4.2 Precipitation kinetics

In the process of the precipitation kinetic simulations more than 70 calculations were executed, but in this chapter only a few of these simulations will be presented. The scripts of the simulations can be seen in the appendix, in the sections G) to CC). The first part comprises standard computations without any additional modifications of the parameters and the corresponding discussion about the results. The second part includes calculations regarding the sensitivity analysis and the last part contains the optimized calculations.

Every precipitation kinetic simulation must be based on a faultless equilibrium phase diagram. Hence, the changed parameters from chapter 4.1.3.2 had to be used for the following simulations, as shown in Table 11.

Table 11: Improved parameters from the equilibrium phase diagram modeling

Parameter	Original value	Modified value
G(LIQUID,AL,SC;0)	273 **-155000**+10*T; 6000 N	273 **-163000**+10*T; 6000 N
G(LIQUID,AL,SC;1)	273 **+20000**; 6000 N	273 **+21300**; 6000 N
G(FCC_A1,AL,SC:VA;0)	273 **-110876**; 6000 N	273 **-112376**; 6000 N

4.2.1 Standard calculations

As mentioned before, the simulations in this section were performed without any modifications of the kinetic parameters. The standard values, which are recommended by MatCalc, are listed in Table 12. The graphical outputs of the most important properties of the precipitates compared with the data from the literature from Table 2 are shown in this chapter.

Table 12: Parameter values of the standard precipitation kinetic simulations

Parameter	Value
Activation Energy *Q**	173000 J/mol
Diffusion pre-exponential factor D_0*	0,000531 m^2/s
Nucleation Constant	1,0
Incubation time Constant	1,0
Inactive Radius Factor	5 %

*For Diffusion of Sc in Al-matrix

4.2.1.1 Precipitate radii

In this part, the outputs of the evolution of the precipitate sizes are plotted. Four calculations, two according to the heat treatments from Marquis [36] and two according to Iwamura [39] are presented. The Figures in this chapter show only the more interesting heat treatment part of aging, where the precipitates are formed and grow. The diagrams present the progressions of the minimum precipitate radius (green line), the maximum precipitate radius (blue line), the mean precipitate radius (cyan line) and the critical precipitate radius (red line). The names in the brackets are the shorthand symbols according to Table 2.

In Figure 34 the precipitate growth during a 120 h aging period at 400 °C is shown, precedent the alloy with an Sc-content of 0,3 wt.% Sc was annealed at 648 °C for 24 h, after Marquis [36].

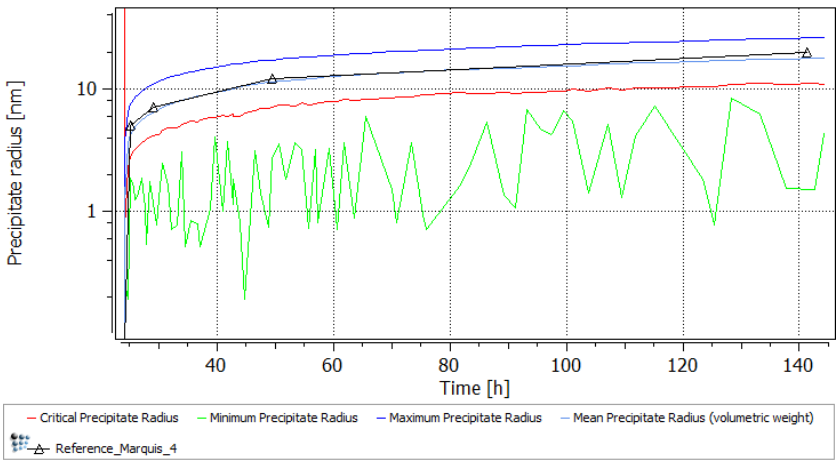

Figure 34: Precipitate radius evolution, based on the heat treatment after Marquis (Marquis_4)

The diagram in Figure 35 also shows a calculation based on the reference values from Marquis [36]. Here, the heat treatment included 24 h annealing at 648 °C and aging at 450 °C for 72 h for an Al-0,3 wt.% Sc alloy.

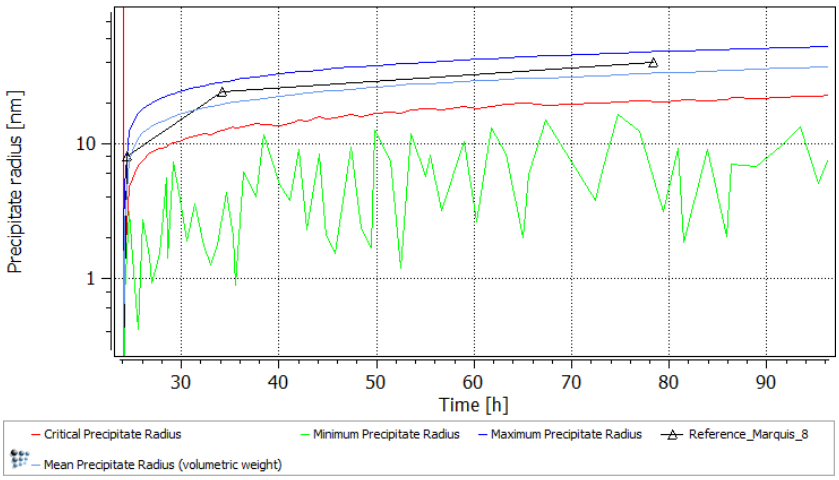

Figure 35: Precipitate radius evolution, based on the heat treatment after Marquis (Marquis_8)

Figure 36 and Figure 37 display the courses of the radii during a long lasting aging of 10^6 s (≈ 280 h) at 400 °C and 490 °C respectively. The not shown annealing period lasted for both 2 h at 640 °C.

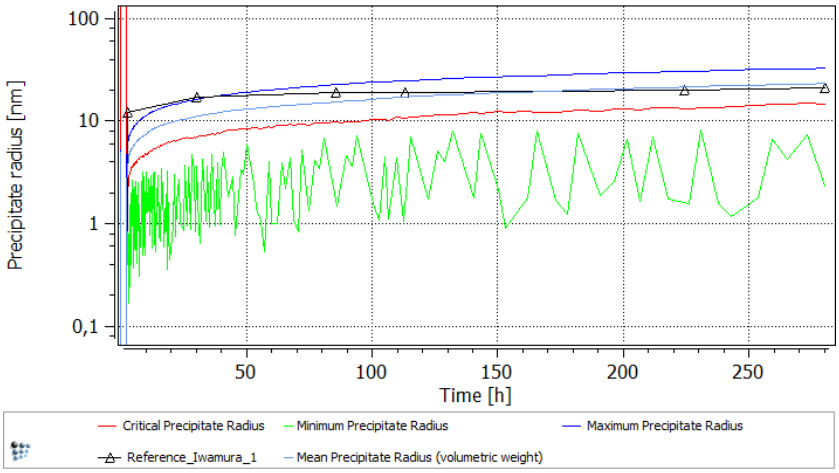

Figure 36: Precipitate radius evolution, based on the heat treatment after Iwamura (Iwamura_1)

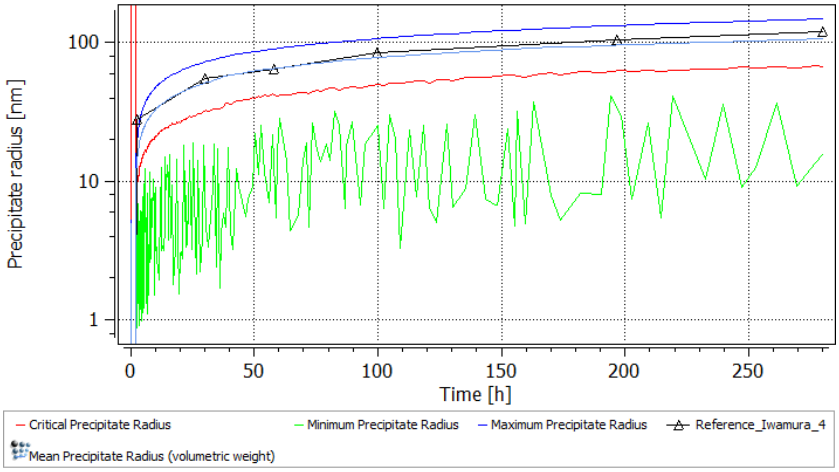

Figure 37: Precipitate radius evolution, based on the heat treatment after Iwamura (Iwamura_4)

4.2.1.2 Phase fraction

The results from the phase fraction simulations are shown in this section, where only the important aging periods are shown which caused for different start times in the diagrams. The first two calculations are based on the inputs of the calculation model of Robson [40], an extension of the N-model. The last two on the heat treatments which were carried out by Royset [13]. Amongst the results (red line), also the reference values (lines with triangle markers) are shown.

Figure 38 is the outcome of a simulated heat treatment of an alloy containing 0,25 wt.% Sc. The alloy was 72 h annealed at 640 °C and aged for 1 h at 450 °C.

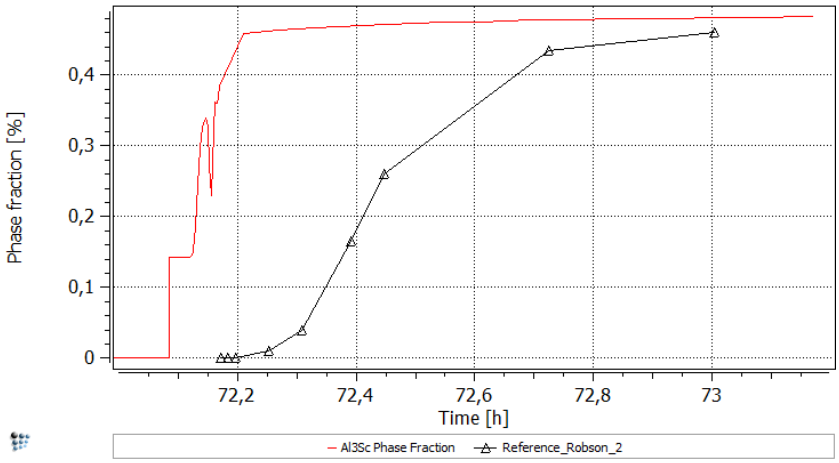

Figure 38: Phase fraction, based on the heat treatment of Robson (Robson_2)

The result of the simulation “Robson_3” is shown in Figure 39, where the alloy with 0,25 wt.% Sc were heat treated at 640 °C for 72 h and for 1 h at 500 °C.

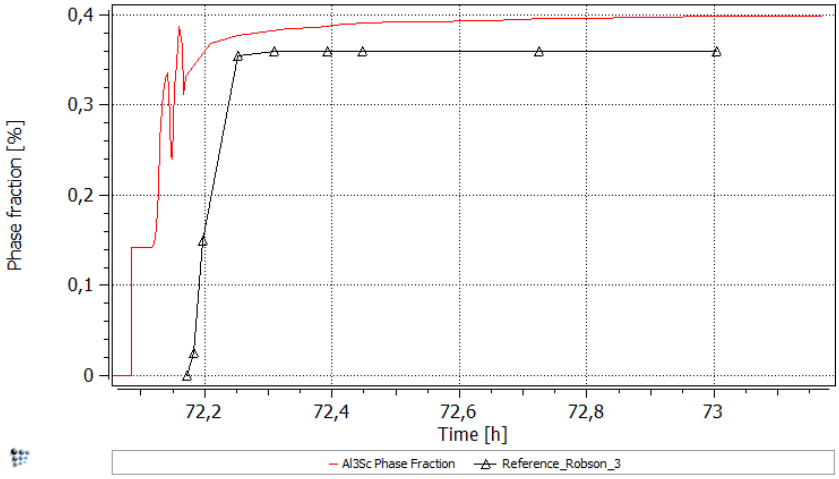

Figure 39: Phase fraction, based on the heat treatment of Robson (Robson_3)

The annealing time for the computations “Royset_1” (Figure 40) and “Royset_2” (Figure 41), was 1 h at a temperature of 600 °C. The aging time was for both 170 h with a temperature of 230 °C for “Royset_1” and 270 °C for “Royset_2”.

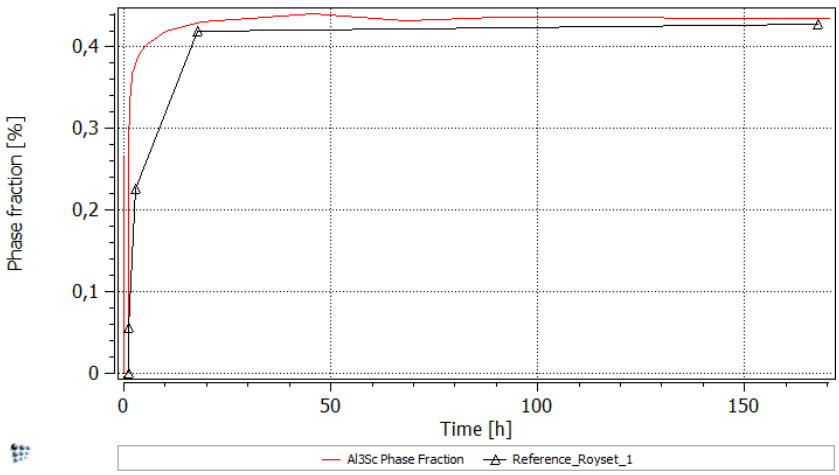

Figure 40: Phase fraction, based on the heat treatment of Royset (Royset_1)

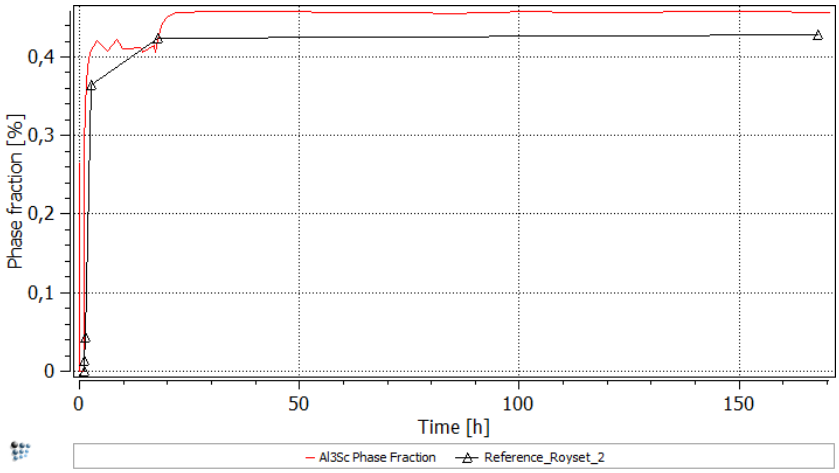

Figure 41: Phase fraction, based on the heat treatment of Royset (Royset_2)

4.2.1.3 Number density

For the computation of the number density only one progression was found in the literature. The calculation is based on an isothermal simulation of Robson [40]. The content of Sc was chosen with 0,11 at.% and the aging temperature was 343 °C. The result (red line), compared with the outcome from Royset (line with triangle markers), is displayed in Figure 42.

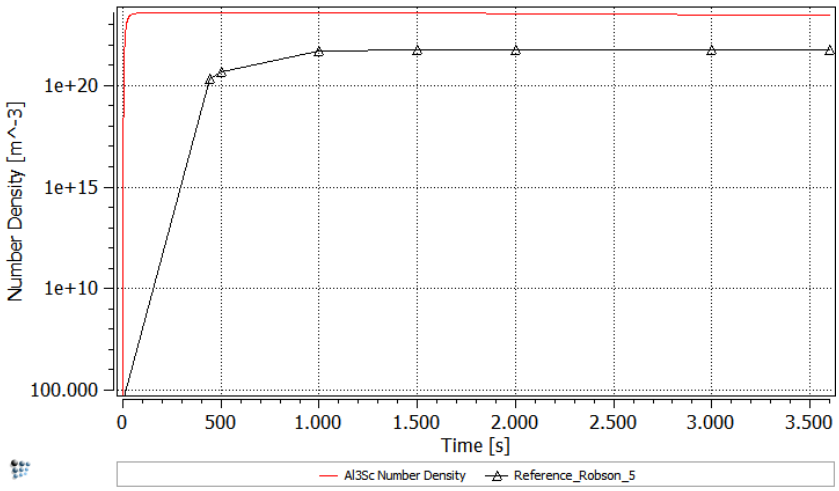

Figure 42: Number density behaviour, based on a isothermal simulation at 343 °C (Robson_5)

4.2.2 Discussion

In Table 13 all results of the standard simulations and their deviations in comparison to the literature data are listed. In this chapter the deviations as seen in the figures which were illustrated in section 4.2.1 are discussed.

Table 13: Results and deviations of the standard precipitation kinetic simulations

Shorthand Symbol	Mean Precipitate Radius from literature [nm]	Phase Fraction from literature	Calculated Precipitate Radius r_{v_mean} [nm]	r_{v_mean} Deviation absolute	r_{v_mean} Deviation [%]	Calculated Phase Fraction	Phase Fraction Deviation absolute	Phase Fraction Deviation [%]
Marquis_1	1	-	1,39	0,39	39,00	0,006800	-	-
Marquis_2	5	0,0097	4,21	-0,79	-15,80	0,006888	-0,002802	-28,92
Marquis_3	5	0,0067	4,20	-0,80	-16,00	0,006483	-0,000257	-3,81
Marquis_4	20	0,0067	17,73	-2,27	-11,35	0,006694	-0,000046	-0,68
Marquis_5	8,8	-	1,84	-6,96	-79,09	0,002200	-	-
Marquis_6	3	-	2,20	-0,80	-26,67	0,004600	-	-
Marquis_7	2	0,0071	2,23	0,23	11,50	0,007009	-0,000051	-0,72
Marquis_8	40	0,0064	37,17	-2,83	-7,07	0,006189	-0,000201	-3,15
Marquis_9	7	-	9,01	2,01	28,71	0,007000	-	-
Marquis_10	3	-	3,14	0,14	4,67	0,007059	-	-
Berezina	5	-	3,43	-1,57	-31,40	0,007100	-	-
Sano	9	-	3,00	-6,00	-66,67	0,005800	-	-
Miura	4	-	8,13	4,13	103,25	0,005300	-	-
Novotny_1	5	0,0069	5,50	0,50	10,00	0,006925	0,000025	0,36
Novotny_2	15	0,0044	18,04	3,04	20,27	0,004640	0,000240	5,44
Iwamura_1	21	-	23,13	2,13	10,14	0,004300	-	-
Iwamura_2	41	-	39,72	-1,28	-3,12	0,004000	-	-
Iwamura_3	76	-	69,26	-6,74	-8,87	0,003700	-	-
Iwamura_4	121	-	107,57	-13,43	-11,10	0,003100	-	-
Robson_1	3,5	-	4,94	1,44	41,14	0,005329	-	-
Robson_2	8,5	0,0046	9,22	0,72	8,47	0,004820	0,000220	4,78
Robson_3	20	0,0036	20,49	0,49	2,45	0,003988	0,000388	10,78
Robson_4	54	0,0023	41,14	-12,86	-23,81	0,002612	0,000362	16,09
Robson_5	-	-	1,56	-	-	0,003900	-	-
Clouet_1	2,5	-	2,98	0,48	19,20	0,007084	-	-
Clouet_2	7	-	7,47	0,47	6,71	0,007007	-	-
Clouet_3	19	-	21,03	2,03	10,68	0,006811	-	-
Royset_1	-	0,0043	0,69	-	-	0,004353	0,000074	1,73
Royset_2	-	0,0043	1,55	-	-	0,004561	0,000282	6,59
Royset_3	-	0,0043	4,83	-	-	0,004597	0,000318	7,43
Royset_4	-	0,0043	11,48	-	-	0,004470	0,000191	4,46

4.2.2.1 Precipitate radii

In chapter 4.2.1.1 the results of the precipitate radii were presented and it is evident that the calculations meet the references appropriately. However, it attracted attention that in all calculations, at the early stage of the precipitation, the deviations are higher than at the end of it.

The final precipitate radii after the heat treatments are listed in Table 13. It was observed that in isothermal calculations, especially "Berezina, Sano, Miura and Clouet_1", as well as calculations with short aging times, like "Marquis_1, Marquis_2, Marquis_3, Robson_1 and Robson_4", the percentage deviations are greater than 15 %. But on closer inspection, it is discernable that the absolute deviation in some calculations are smaller than 2 nm, which is a good approximation.

4.2.2.2 Phase fraction

The data from the final results of the phase fraction also show a good comparison with the ones from the literature, where the computations have deviations below 10 %. However, the calculations "Marquis_2, Robson_3 and Robson_4" have larger deviations, whereby only the deviation of "Marquis_2" is higher than 20 %.

The developments of the phase fractions in section 4.2.1.2 show some irregularities in the areas, where the precipitation comes to an equilibrium. Furthermore, it was observed that the simulations of Robson regarding the start of the nucleation, have a delay of approximately 10 minutes. The results of the calculations show in Figure 40 and Figure 41 that the start of the nucleation is 2 minutes too early.

4.2.2.3 Number density

In Figure 42, it is apparent that the enlargement of the number density is too steep and does not match the graph from the literature. Additional, the calculated end-result is much too high and extremely overestimated by MatCalc. Table 14 confirms the overestimation with the results of the calculations of Marquis.

Table 14: Results and deviations of the number density calculation

Shorthand Symbol	Literature Data [m^{-3}]	Calculated [m^{-3}]	Deviation absolute [m^{-3}]	Deviation [%]
Marquis_5	$7 \cdot 10^{20}$	$9{,}23 \cdot 10^{22}$	$9{,}16 \cdot 10^{22}$	13086
Marquis_6	$1{,}1 \cdot 10^{22}$	$1{,}37 \cdot 10^{23}$	$1{,}26 \cdot 10^{23}$	1145
Marquis_7	$6 \cdot 10^{22}$	$1{,}97 \cdot 10^{23}$	$1{,}37 \cdot 10^{23}$	228
Robson_5	$5{,}7 \cdot 10^{21}$	$2{,}75 \cdot 10^{23}$	$2{,}69 \cdot 10^{23}$	4725

4.2.2.4 Summary

Generally, it has been found that

- The precipitate growth is in good agreement to the references
  In the presented precipitate radius evolutions in chapter 4.2.1.1 it can be seen that the calculated graphs only in the earlier stages of precipitation do not match with the ones from the references. The final precipitate sizes are in the area of the experiments and showing a mean deviation of 20,56 %.

- The equilibrium phase fractions are partially reached too quickly
  In comparison to experimental data from Royset [13], the nucleation starts at the right time and the equilibrium phase fraction is reached too quickly. In comparison to the results of the simulations from Robson [40] the graphs appear such that the nucleation starts to early, but all the other simulations related to experimental data starting at the right time, which led to the conclusion that the simulations of Robson [40] is delayed. This can be seen in the figures of section 4.2.1.2.

- The final phase fractions are too high
  The final values show a standard deviation of 7,4 %, so it is possible to neglect the outlier "Marquis_2", because values above four times the standard deviation should be neglected. This results in a mean deviation of 5,08 % for the final phase fractions (Table 13).

- The nucleation rates are too high
  As seen in Figure 42, the slope between the time of 0 and 500 s, which signifies the nucleation rate, is too steep in comparison to the reference graph.

- The final number densities are too high
  Apparent in Figure 42 and Table 14, the final number density is up to 130 times bigger than the references.

4.2.3 Sensitivity analyses

Due to the large deviations in the number density simulation, it is necessary to change the parameters, which are mentioned in Table 12. To accumulate information on how the parameters influences the calculations, a sensitivity analysis was performed. Afterwards, the changed parameters were applied to all simulations and then the outputs were investigated again. In this chapter the results of the analyses are presented.

4.2.3.1 Activation energy of diffusion

The activation energy of diffusion *Q* which is also called energy barrier and influences the nucleation through the relationship of the diffusion coefficient for Sc in the Al-matrix

$$\boldsymbol{D = D_0 * exp(-\frac{Q}{RT})}, \qquad \textbf{eq. 4.1}$$

where the exponential function indicates the probability that an atom leaves its original position, with *R* as the ideal gas constant and *T* describing the absolute temperature and D_0 is the pre-exponential factor.

In Figure 43 it is apparent that an increase of the energy barrier leads to a later start of the nucleation which causes a significant decrease of the nucleation rate. The nucleation was finished later at a lower amount of precipitates and the growth and coarsening will also start later, which is not shown in the diagram.

The standard value for the activation energy of diffusion is 173000 J/mol, Figure 44 shows that an increase of 23250 J/mol gives a good approach for the start of the nucleation but does not meet the remaining reference number density course of Robson. Also the start of the nucleation agrees with the reference without large deviations.

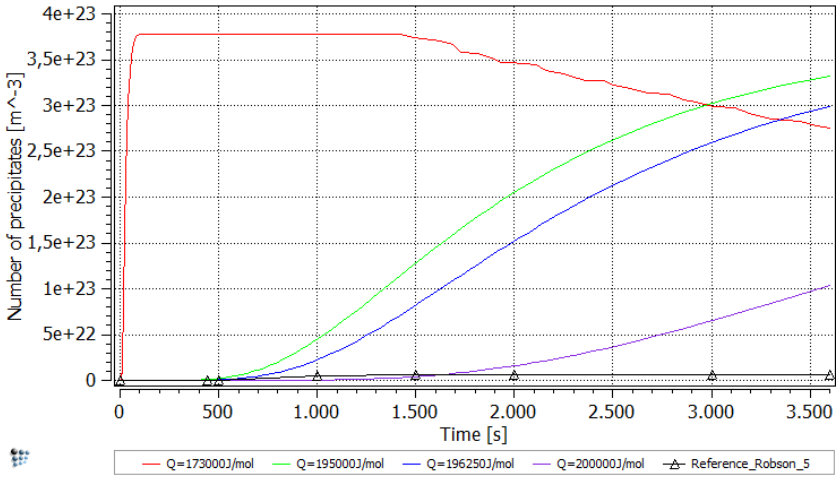

Figure 43: Sensitivity analysis of the activation energy

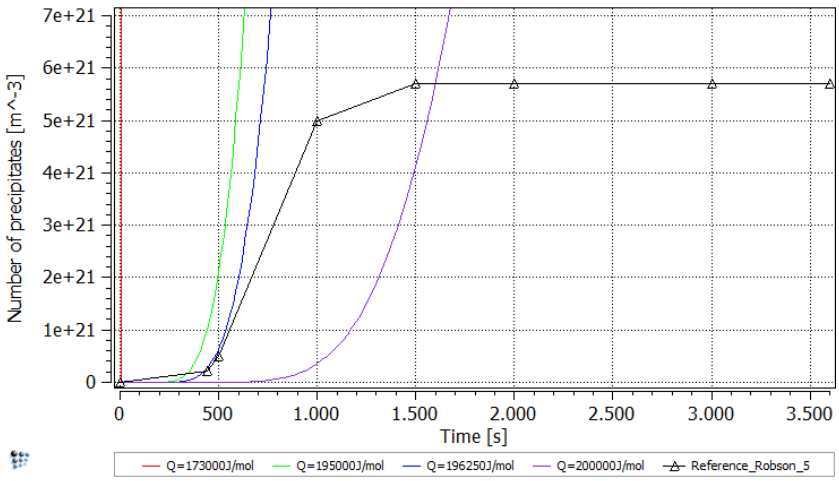

Figure 44: Detailed view of the sensitivity analysis of the activation energy

4.2.3.2 Diffusion pre-exponential factor

As mentioned in eq.4.1, also the pre-exponential factor influences the diffusion coefficient and further the nucleation and growth. A doubling of the factor leads to a faster nucleation rate, a slightly increase of the number of new formed nuclei and an earlier start of the coarsening, which reduces the final number density. Figure 45 also shows that a further increase of the pre-exponential factor results in a minimization of the growth period and an immediate start of the coarsening. The nucleation rate was increased and after the nucleation is finished, the number of precipitates drops down. As presented in Figure 46 the final number density at higher pre-exponential factors is lower than the one from the reference, but the shape of the curves is completely different. This fact concludes that this change is not practical and do not deserve an appropriate result. The standard pre-exponential factor is denoted with 0,000531 m^2/s by MatCalc and will remain in the optimization.

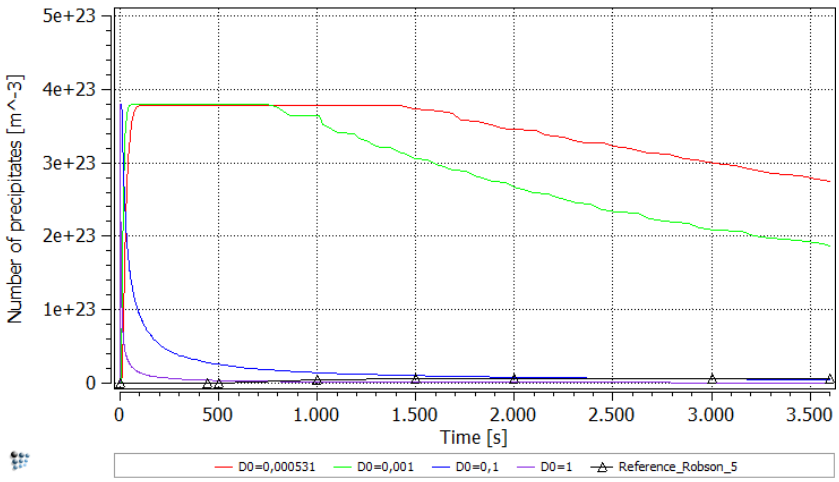

Figure 45: Sensitivity analysis of the diffusion pre-exponential factor

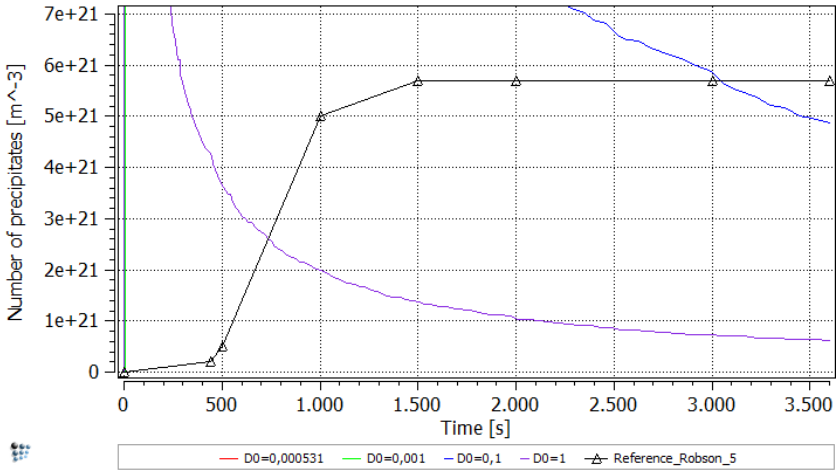

Figure 46: Detailed view of the sensitivity analysis of the diffusion pre-exponential factor

4.2.3.3 Incubation time constant

The incubation time constant is equivalent with the incubation time τ from eq. 2.10, the transient nucleation rate, and has according to MatCalc a standard value of 1,0. An increase of the incubation time constant leads to a slower nucleation rate and a later start of the growth and coarsening, which results in trends with the appearance of the reference curve. A decrease of the factor has an effect in the opposite direction. Higher incubation time constants (> 100) lower the final number density significantly, but delay the nucleation. In Figure 47 simulations with different incubation time constants are plotted. Figure 48 gives a detailed view of the number density progressions for higher incubation time constants.

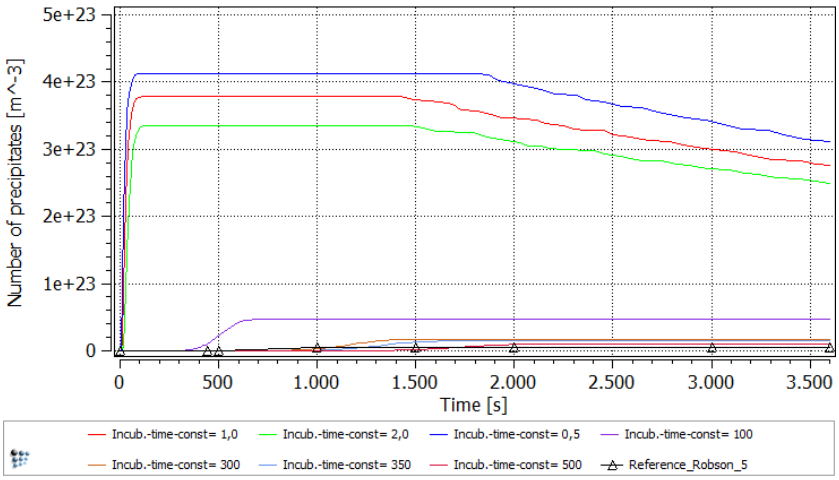

Figure 47: Sensitivity analysis of the incubation time constant

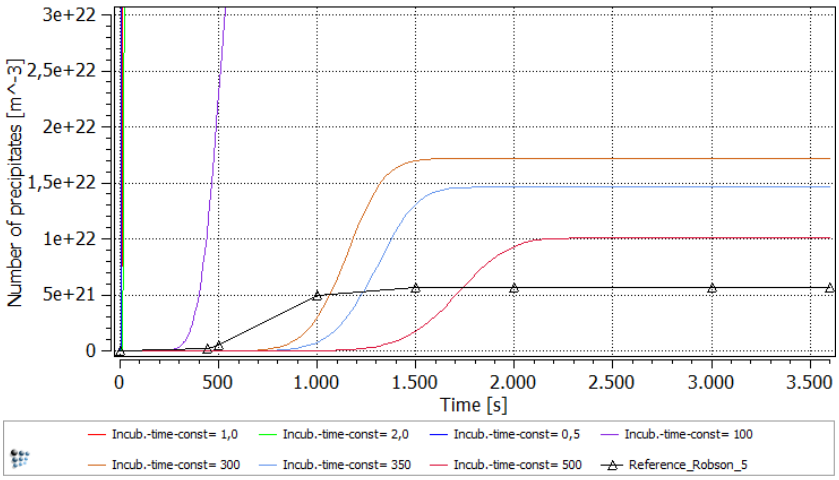

Figure 48: Detailed view of the sensitivity analysis of the incubation time constant

4.2.3.4 Nucleation constant

A lower nucleation constant decreases the final number of precipitates, as well as the nucleation rate, displayed in Figure 49. To achieve the final number density of the reference, the nucleation constant had to be decreased from the standard value 1,0 to 0,000125, if no other parameter is changed. The changes of the constant did not affect the early start of the nucleation and small variations led to a slight decrease of the nucleation rate, as shown in Figure 50.

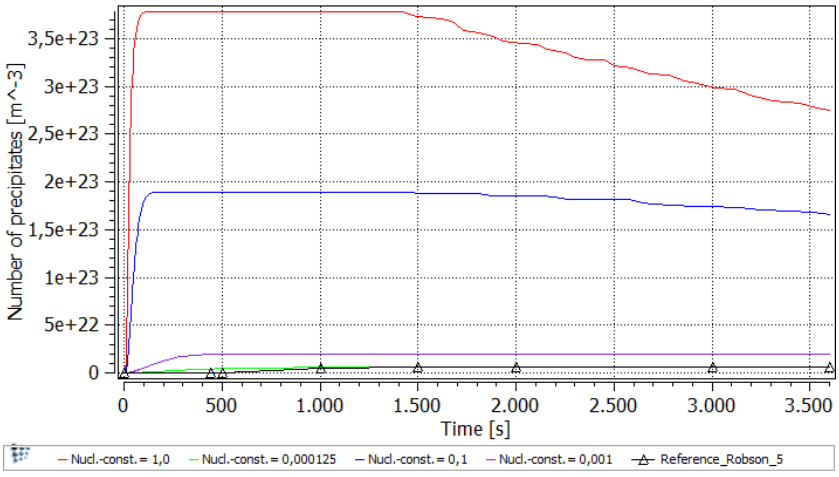

Figure 49: Sensitivity analysis of the nucleation constant

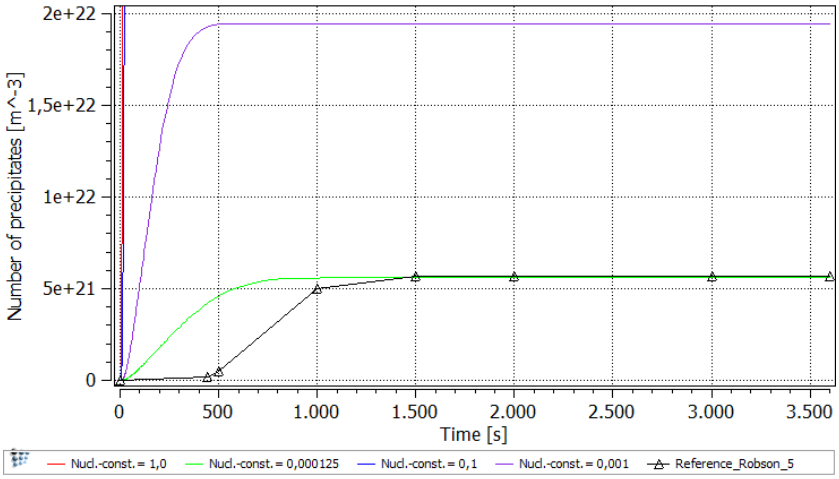

Figure 50: Detailed view of the sensitivity analysis of the nucleation constant

4.2.3.5 Inactive radius factor

The inactive radius factor defines an area around a precipitate, where new precipitates are restricted to nucleate. It is related to the actual precipitate radius in percentage and the standard value is 5, suggested by MatCalc. A higher inactive radius factor leads to less space for nucleation and therefore decreases the nucleation rate and the final number of precipitates. Figure 51 shows the different variations of the inactive radius factor, and it is apparent that the start of the nucleation is not influenced.

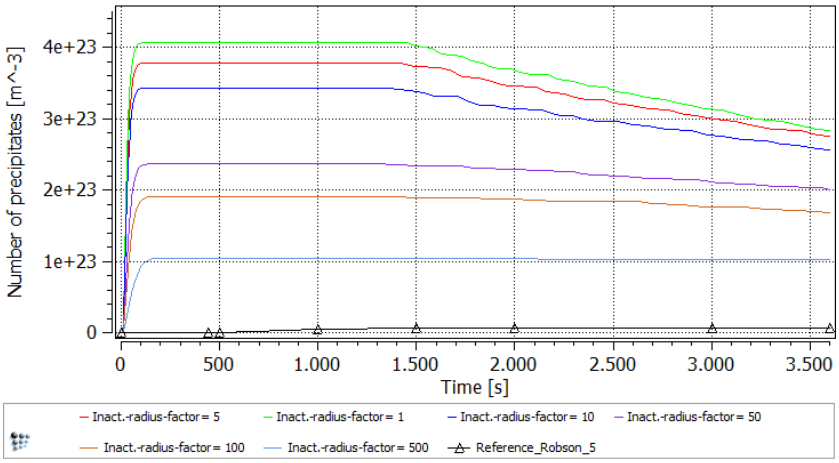

Figure 51: Sensitivity analysis of the inactive radius factor

4.2.4 Optimized calculations

Based on the results from the sensitivity analysis and the optimization of the equilibrium phase diagram, it was possible to modify the parameters to gather a calculation model, which improved the results of the precipitation kinetic simulations.

Table 15: Changed parameters of the optimized precipitation kinetics simulation

Parameter	Original value	Modified value
G(LIQUID,AL,SC;0)	273 **-155000**+10*T; 6000 N	273 **-163000**+10*T; 6000 N
G(LIQUID,AL,SC;1)	273 **+20000**; 6000 N	273 **+21300**; 6000 N
G(FCC_A1,AL,SC:VA;0)	273 **-110876**; 6000 N	273 **-112376**; 6000 N
MQ(FCC_A1&SC,AL:VA;0)	273 **-173000**+R*T*LN(+0,000531); 6000 N	273 **-169000**+R*T*LN(+0,000531); 6000 N
Incubation time constant	1,0 s	500 s
Inactive radius factor	5	50

In Table 15 all changed parameters for the optimized simulation listed. The first three parameters were already described in Table 4 and were not changed again. MQ(FCC_A1&SC,AL:VA;0) denotes the diffusion coefficient of Al in an Al-matrix with solved Sc and is represented in eq. 4.1 in the transformed statement

$$\boldsymbol{RT * lnD = -Q + RT * lnD_0,} \qquad \textbf{eq. 4.2}$$

where the symbols are the same as in chapter 4.2.3.1. Q was decreased by 4000 J/mol and D_0 was kept by its standard value. Additionally, the incubation time constant was increased to 500 and the inactive radius factor was enlarged to 50.

As in chapter 4.1, the following diagrams show only the important parts of the aging period according to the heat treatments of Table 2.

4.2.4.1 Precipitate radii

As result of the optimization, the curves of the precipitate radii are now steeper as before and the final radii are larger. If the deviations in the standard calculations were negative, the new deviations are smaller now or low positive. Previous positive deviations were also extended. During the optimization, the main focus was set on the number density, in consequence of the big variances in the standard calculations (> 130 times). This led to a less concurrent progress of the precipitate radii.

Figure 52 shows the result from the optimized calculation of “Marquis_4”. It is apparent that the calculated curve is almost parallel to the references with a difference of approximately 1,4 nm during the aging and an absolute difference of 2,1 nm for the final precipitate radius.

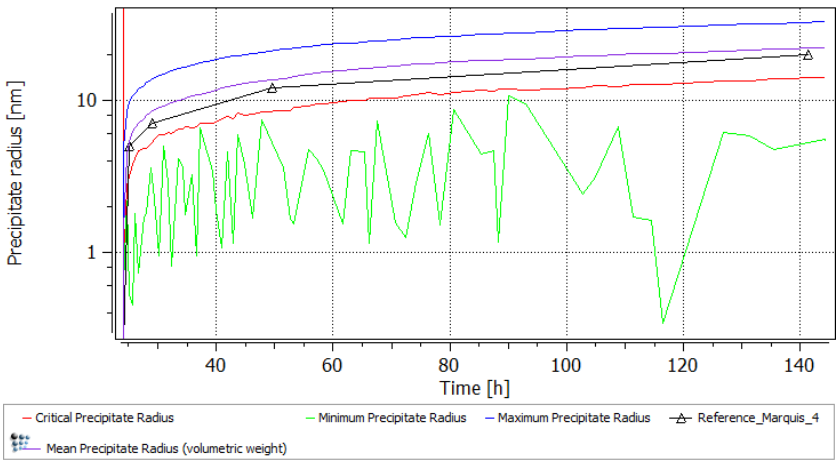

Figure 52: Optimized precipitate radius evolution, based on the heat treatment of Marquis (Marquis_4)

The optimized calculation of “Marquis_8”, plotted in Figure 53, shows the same alteration. The mean precipitate radius curve is now in good convergence to the reference, but the final value has now a positive deviation of 5,09 nm in comparison to the first calculated deviation of -2,83 nm.

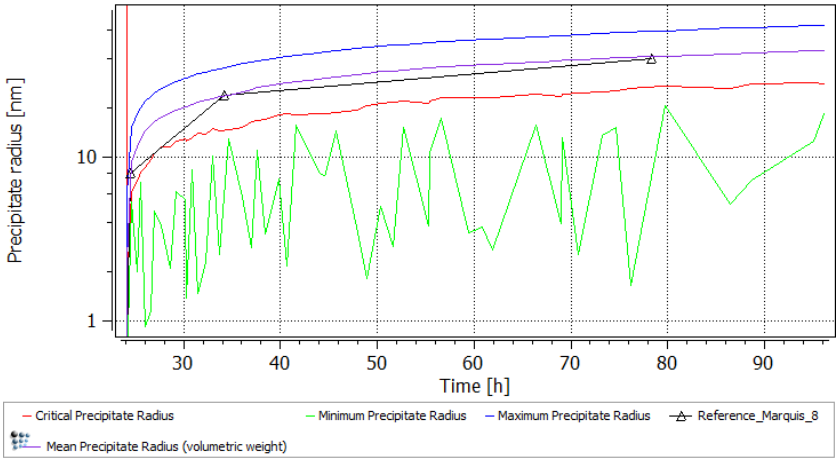

Figure 53: Optimized precipitate radius evolution, based on the heat treatment of Marquis (Marquis_8)

Also the modified calculation of “Iwamura_1” appears with larger deviations as before. Almost the whole evolution of the mean radius is now above the reference, as shown in Figure 54. The final mean radius has an absolute deviation of 7,81 nm instead of 2,13 nm.

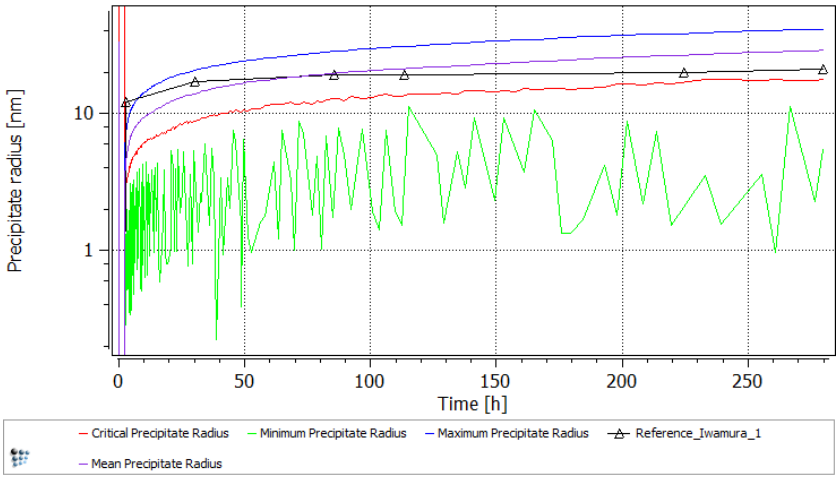

Figure 54: Optimized precipitate radius evolution, based on the heat treatment of Iwamura (Iwamura_1)

The optimized calculation of "Iwamura_4" shows an improvement of the final precipitate radius, where the absolute deviation was -13,43 nm before the modification and now it is 10,19 nm. As in the previous optimized calculations, the progression of the mean precipitate radius appears now higher in the whole range of the aging, which can be seen in Figure 55.

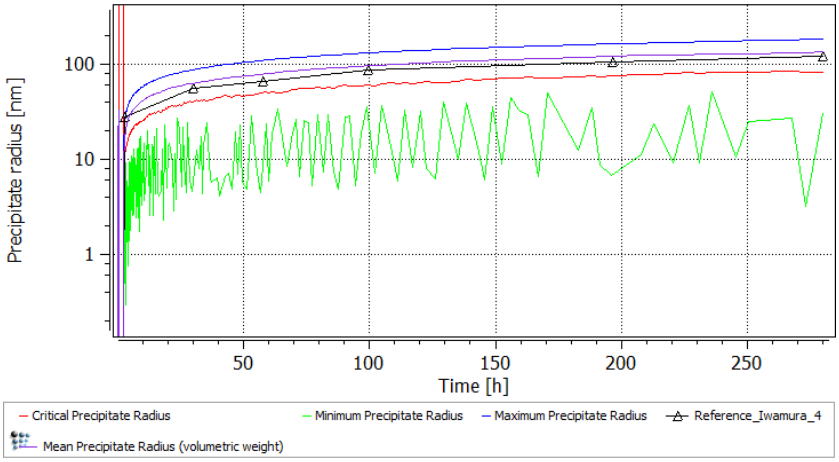

Figure 55: Optimized precipitate radius evolution, based on the heat treatment of Iwamura (Iwamura_4)

4.2.4.2 Phase fraction

The optimization affected the phase fraction same way, as seen at the precipitate radii. The most final deviations of the phase fractions were slightly enlarged. The progressions stayed nearly the same.

Figure 56 shows the optimized phase fraction course of "Robson_2", which almost remained the same. The deviation of the final phase fraction was little enlarged from 4,78 % up to 5,67 % and the irregularities during the nucleation were reduced, but it was not possible to remove the plateau at

72,1 h. The difference at the start of the nucleation is on account of the simulation of Robson, in comparison to experimental data the nucleation starts in all other calculations at the right time.

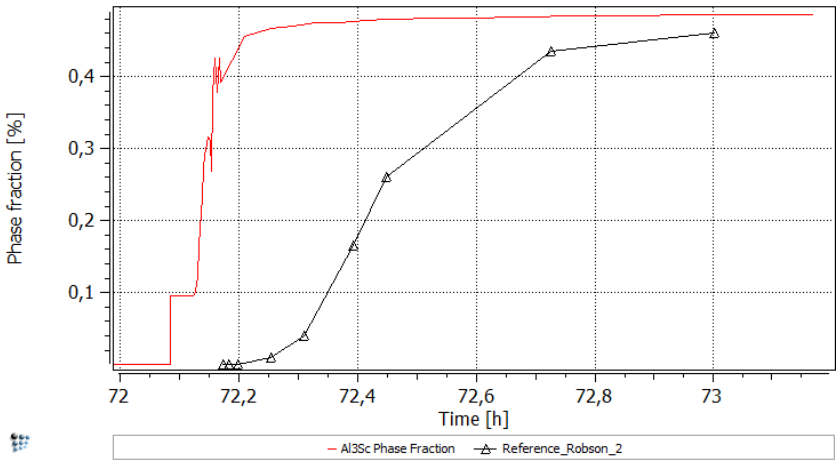

Figure 56: Optimized phase fraction, based on the heat treatment of Robson (Robson_2)

The next calculation, shown in Figure 57, is also based on the heat treatments of Robson, the deviations at the start of the aging period are the same. In this simulation the unevenness could not be reduced, and the final phase fraction deviation was even increased from 10,78 % to 11,64 %.

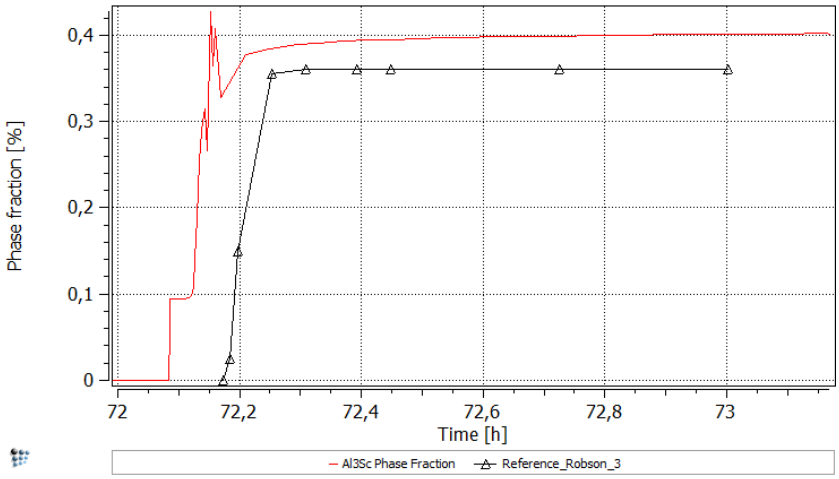

Figure 57: Optimized phase fraction, based on the heat treatment of Robson (Robson_3)

The diagrams in Figure 58 and Figure 59 are showing the calculations according to “Royset_1” and “Royset_2”, respectively. The curves remained nearly the same, but the irregularities of “Royset_2” were intensified. The deviations of the final phase fraction were on the one hand for Royset_1 decreased and on the other hand for “Royset_2” increased. The initial variance of “Royset_1” were lowered from 1,73 % to 1,61 % and “Royset_2” experienced an enlargement from 6,59 % to 10,03 %.

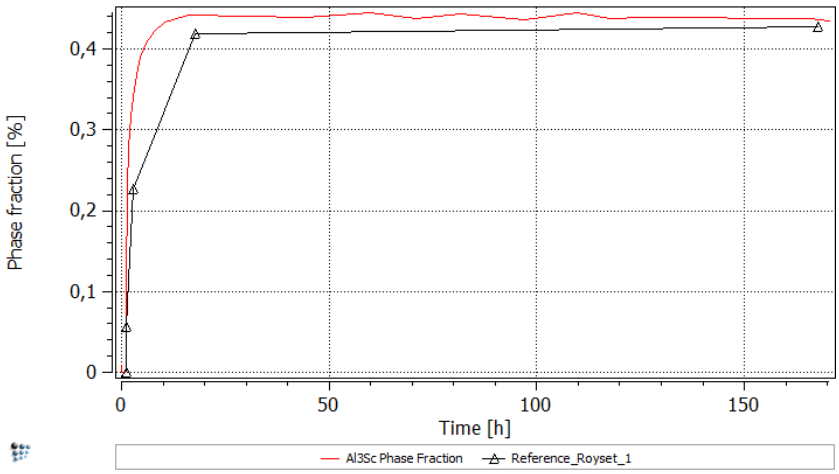

Figure 58: Optimized phase fraction, based on the heat treatment of Royset (Royset_1)

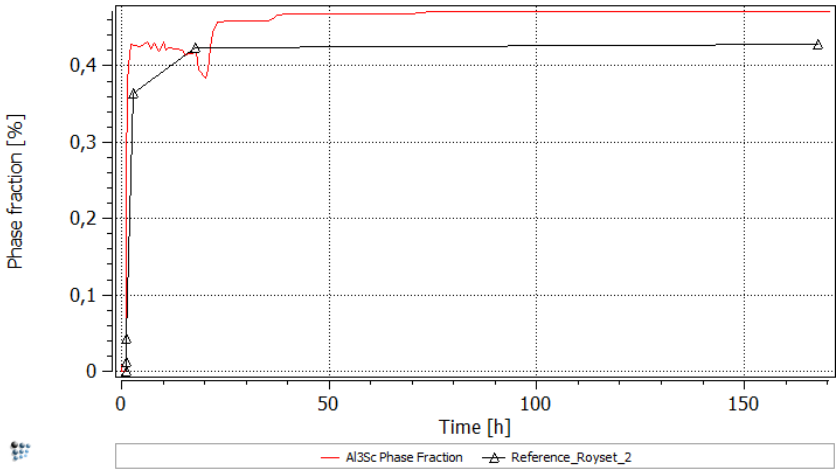

Figure 59: Optimized phase fraction, based on the heat treatment of Royset (Royset_2)

4.2.4.3 Number density

As already mentioned the focus of the optimization was on the number density, which is the reason for the good conformity of the number density progression with the reference in Figure 60. The final number densities and their according deviations are listed in Table 16. In comparison with Table 14, it is evident that the variances are decreased in an adequate scale. It was possible to minimize the deviation of “Marquis_5” from 13086 % to 375 %, but also the other calculations, especially “Robson_5”, were optimized appropriately. The optimization of the number density also influenced the nucleation rate, which has been reduced drastically.

Table 16: Results and deviations of the optimized number density calculation

Shorthand Symbol	Literature Data [m^{-3}]	Calculated [m^{-3}]	Deviation absolute [m^{-3}]	Deviation [%]
Marquis_5	$7 \cdot 10^{20}$	$3{,}33 \cdot 10^{21}$	$2{,}63 \cdot 10^{21}$	375,23
Marquis_6	$1{,}1 \cdot 10^{22}$	$2{,}23 \cdot 10^{22}$	$1{,}13 \cdot 10^{22}$	102,93
Marquis_7	$6 \cdot 10^{22}$	$1{,}10 \cdot 10^{23}$	$4{,}97 \cdot 10^{22}$	82,80
Robson_5	$5{,}7 \cdot 10^{21}$	$5{,}62 \cdot 10^{21}$	$-8{,}44 \cdot 10^{19}$	-1,48

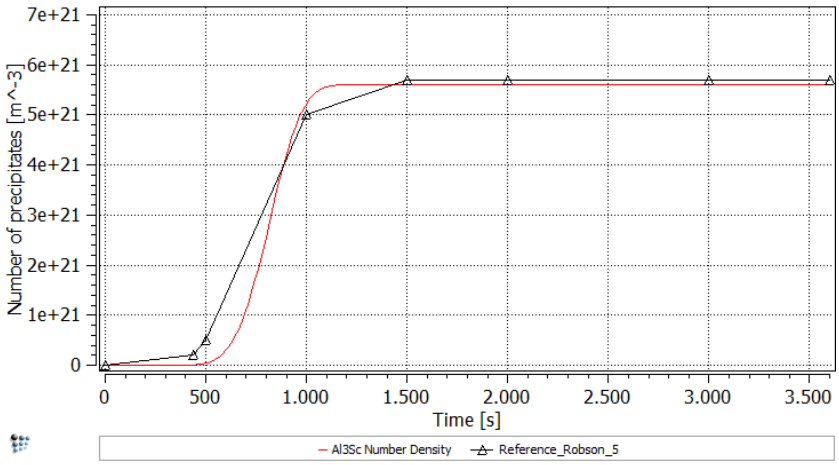

Figure 60: Optimized number density evolution, based on a isothermal simulation at 343 °C (Robson_5)

4.2.4.4 Summary

In summary, the optimization influenced the results in comparison to the standard precipitation kinetic simulations as followed:

- The final precipitate sizes were enlarged in all calculations.
- The growth rates during aging were also increased in every calculation.
- The final phase fractions stayed the same in most calculations. The results of two calculations were slightly decreased and in 14 calculations the final phase fractions were increased.
- The equilibrium phase fractions were still reached too early.
- The final number density was decreased drastically.
- Nucleation rates were decreased to a better matching scale in every calculation.

In sake of completeness, the results and deviations of all optimized precipitation kinetic simulations are illustrated in Table 17. The shorthand symbols are still dependent to Table 2.

Table 17: Results and deviations of the optimized precipitation kinetic simulations

Shorthand Symbol	Mean Precipitate Radius from literature [nm]	Phase Fraction from literature	Calculated Precipitate Radius r_{v_mean} [nm]	r_{v_mean} Deviation absolute	r_{v_mean} Deviation [%]	Calculated Phase Fraction	Phase Fraction Deviation absolute	Phase Fraction Deviation [%]
Marquis_1	1	-	1,65	0,65	65,00	0,006800	-	-
Marquis_2	5	0,0097	5,26	0,26	5,20	0,006917	-0,002773	-28,62
Marquis_3	5	0,0067	5,40	0,40	8,00	0,006484	-0,000256	-3,80
Marquis_4	20	0,0067	22,10	2,10	10,50	0,006694	-0,000046	-0,68
Marquis_5	8,8	-	5,70	-3,10	-35,23	0,002200	-	-
Marquis_6	3	-	4,04	1,04	34,67	0,004600	-	-
Marquis_7	2	0,0071	2,79	0,79	39,50	0,007009	-0,000051	-0,72
Marquis_8	40	0,0064	45,09	5,09	12,73	0,006189	-0,000201	-3,15
Marquis_9	7	-	11,28	4,28	61,14	0,007000	-	-
Marquis_10	3	-	3,18	0,18	6,00	0,007066	-	-
Berezina	5	-	4,60	-0,40	-8,00	0,007100	-	-
Sano	9	-	4,16	-4,84	-53,78	0,005800	-	-
Miura	4	-	11,15	7,15	178,75	0,005300	-	-
Novotny_1	5	0,0069	7,12	2,12	42,40	0,006925	0,000025	0,36
Novotny_2	15	0,0044	23,38	8,38	55,87	0,004646	0,000246	5,59
Iwamura_1	21	-	28,81	7,81	37,19	0,004300	-	-
Iwamura_2	41	-	50,20	9,20	22,44	0,004000	-	-
Iwamura_3	76	-	82,95	6,95	9,14	0,003700	-	-
Iwamura_4	121	-	133,33	12,33	10,19	0,003100	-	-
Robson_1	3,5	-	5,19	1,69	48,29	0,005317	-	-
Robson_2	8,5	0,0046	11,63	3,13	36,82	0,004861	0,000261	5,67
Robson_3	20	0,0036	25,04	5,04	25,20	0,004019	0,000419	11,64
Robson_4	54	0,0023	48,89	-5,11	-9,46	0,002634	0,000384	17,08
Robson_5	-	-	5,75	-	-	0,003999	-	-
Clouet_1	2,5	-	4,16	1,66	66,40	0,007106	-	-
Clouet_2	7	-	9,94	2,94	42,00	0,007020	-	-
Clouet_3	19	-	27,01	8,01	42,16	0,006819	-	-
Royset_1	-	0,0043	0,77	-	-	0,004348	0,000069	1,61
Royset_2	-	0,0043	2,14	-	-	0,004708	0,000429	10,03
Royset_3	-	0,0043	6,24	-	-	0,004612	0,000333	7,78
Royset_4	-	0,0043	13,61	-	-	0,004480	0,000201	4,70

5. Final Discussion

The results of the equilibrium phase diagram modeling show a very accurate equilibrium phase diagram. The changes of the parameters were minimal invasive, debugged the calculation and lead to temperature deviations smaller than 5 % in the range between 0 – 30 wt.% Sc. In the most important area of the equilibrium phase diagram, at a Sc-concentration between 0,1 – 3,3 wt.%, the deviations of the temperature were even smaller, under 2,5 %. The phase boundaries and the eutectic point are lying on the right positions and the phase areas are well defined.

The optimization of the precipitation kinetics led to modifications of all relevant precipitate properties and their progression during aging.

The progressions of the precipitate size appear after the optimization slightly higher than the reference radii from the literature. Besides, the course of the mean radii shows no irregularities, e.g. jumps or drops and the growth rate is also slightly too high. An observation of the final precipitate radii revealed that the maximum percentage deviation is 178,75 %, which equals 7,15 nm for the calculation “Miura” and the maximum absolute deviation is 21,33 nm, which is equal to 10,19 % for the calculation “Iwamura_4”. Apart from that, the minimum deviation is 0,18 nm or 6,00 % for the calculation “Marquis_10”. A mean deviation of 31,49 % was calculated, which is an increase of 10, 94 %. The reason for the increase derives most likely from the fact, that the optimization is based on four calculations and this circumstance led to two conclusions, whereby one of these is in minimum true:

1.) The optimizations are not applicable on all calculations.
2.) The measurements of the number densities are inaccurate in particular.

All results of the precipitate radii calculations are graphically plotted in Figure 61 and compared to the literature data, where it is apparent that the introduced simulation model is able to meet the experimental values in the whole range.

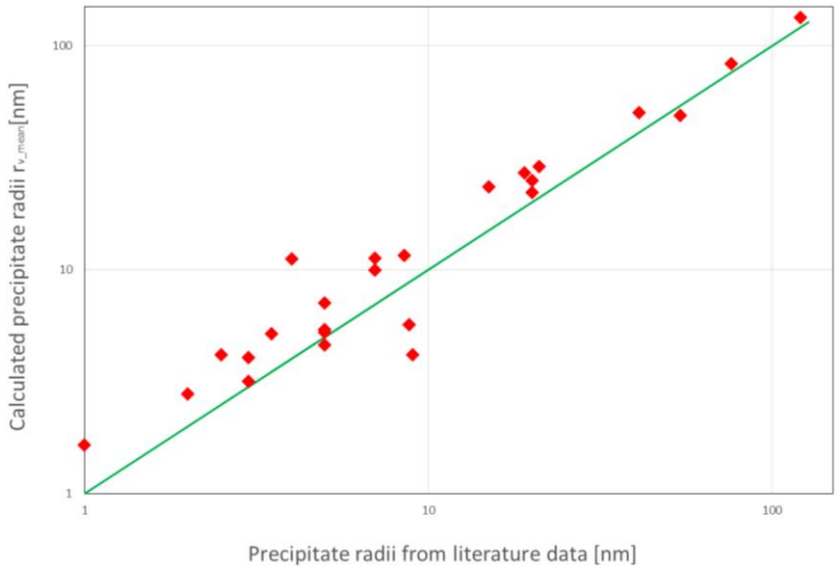

Figure 61: Graphical comparison of the final precipitate radii with the literature data

The phase fraction calculations, based on experimental data, show a too strong ascent during the initial period of the aging. The afterwards reached equilibrium phase fraction is also too high and the transition to it occurs too fast. A closer look on calculations, based on simulations from literature, shows irregularities in the slope increase as well as in the transition area to the equilibrium phase fraction. The investigations also showed that the simulation of Robson [40] has a start delay, which did not appear in calculations with experimental references. The deviations of the final phase fractions are between a maximum of 28,62 % (Marquis_2) and a minimum of 0,36 % (Novotny_1), which equals 0,002773 and 0,000025 in absolute values. In Figure 62 the results of the final phase fractions, compared with the values from the literature data, shows a good concordance, except of one outlier. The outlier is the result of the simulation “Marquis_2”, with the just mentioned maximum deviation. It was observed that this calculation was not influenced by the optimization and the reason for the large deviation could be among other a faulty measurement.

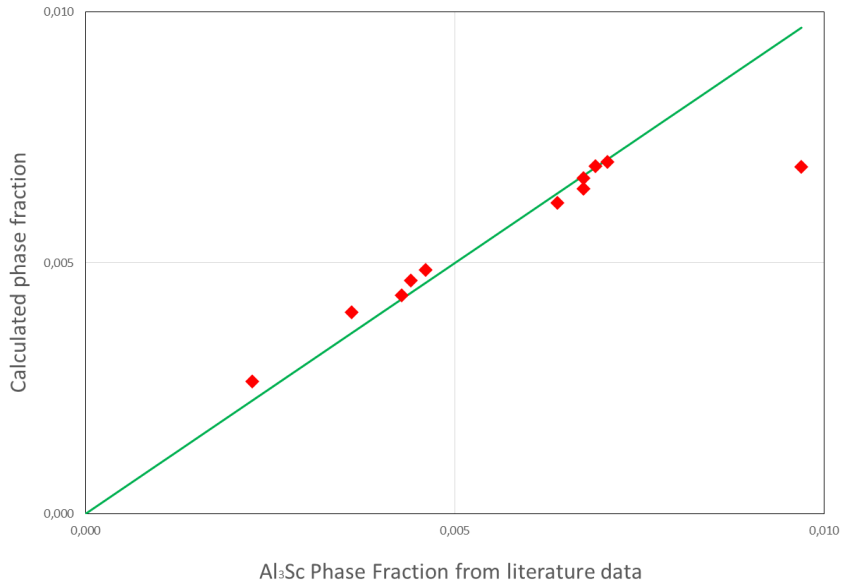

Figure 62: Graphical comparison of the final phase fraction with the literature data

The high deviations in the calculations of the number density were decreased by the optimization. The calculation “Marquis_5” improved from a deviation of 13086 % to 375,23 % and the other calculations behaved the same. However, it was possible to decrease the deviation of “Robson_5” from 4725 % to 1,48 %. The progression of the number density shows no irregularities during aging, but the nucleation rate appears too high. The start of the nucleation is delayed, which could have caused the higher nucleation rate. Also, at the investigated phase fraction progression, the transition to the equilibrium number density comes too abrupt, which is attributed to the direct influence of the number density on the phase fraction.

6. Conclusion & Outlook

In this work, the thermodynamic database of Al and Sc were optimized to gather a well-placed and correct equilibrium phase diagram. This builds the basis for further simulations and calculations in MatCalc for this alloy system, e.g. thermo-mechanical treatments or precipitation strengthening simulations.

Furthermore, with the obtained modifications of the thermodynamic database parameters, it was possible to carry out an optimization of the diffusion database of Al and Sc. This led to an approximation for the evolutions of the precipitate, the phase fraction and the number density. These quantities could act as clue for the design of experiments for new Al-Sc alloys.

The next step for an accurate simulation of precipitation kinetics, will be the refinement of the parameter changes to reach a better convergence of the property progressions and to lower the deviations of the final results. It is also recommended to make investigations on the irregularities in the phase fraction evolutions and on the improvement of the nucleation rate, which also appears too high. A further area of investigation could be the number density distribution of the precipitates and to improve the databases further if necessary.

In the near future, thoughts should be made about the integration of additional elements, e.g. Mg and Zr, to calculate ternary or quaternary alloy systems, which can be of big interest for the aerospace industries.

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8. List of Figures

9. List of Tables

10. Appendix

A) Script of the equilibrium phase diagram modeling without any database changes

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Modeling of the equilibrium phase diagram without any parameter changes
$Database: mc_al.v2.001.tdb
$Author: René Wang
$Date of creation: 2016-10-12
$MatCalc version 5.60
$MatCalc-file name: Al-Sc_eq-phase-diagram_original.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t wt.% Sc           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 1 a y 1 t Temperature [°C]      $defines y-axis title
set-plot-option 1 G M X Y                       $displays grid of x-axis
set-plot-option 1G M Y Y                        $displays grid of y-axis
set-plot-option 1 s n b t$c                     $define series
set-plot-option 1 s m 0 FCC_Al                  $names the series
$*****************************************************************************************
$CALCULATION OF THE Al-MATRIX BOUNDARY
$*****************************************************************************************
set-temperature-celsius 800                     $defines start temperature
set-automatic-startvalues                       $sets automatic start values
calculate-equilibrium                           $calculates equilibrium for set temperature
search-phase-boundary t fcc_a1                  $defines and executes the search for the
                                                $phase boundary
set-step-option y p                             $defines the type of the stepped
                                                $equilibrium calculation
set-step-option r 0.00005 30 l 0.05             $defines the range of the calculation, the
                                                $increment and the interval type
set-step-option e sc                            $defines the varying element
```

```
set-step-option p fcc_a1                    $defines target phase
step-equilibrium                            $executes stepped equilibrium calculation
set-plot-option 1 s d 0                     $locks and duplicates fcc_a1
set-plot-option 1 s m 1 Liquid              $Renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE LIQUID PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                 $defines start temperature
calculate-equilibrium                       $calculates equilibrium for set temperature
search-phase-boundary t liquid              $defines and executes the search for the
                                            $phase boundary
set-step-option p liquid                    $defines target phase
step-equilibrium                            $executes stepped equilibrium calculation
set-plot-option 1 s d 1                     $locks and duplicates liquid
set-plot-option 1 s m 2 Al3Sc_sec           $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_sec PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                 $defines start temperature
calculate-equilibrium                       $calculates equilibrium for set temperature
search-phase-boundary t al3sc               $defines and executes the search for the
                                            $phase boundary
set-step-option p al3sc                     $defines target phase
step-equilibrium                            $executes stepped equilibrium calculation
set-plot-option 1 s d 2                     $locks and duplicates Al3Sc_sec
set-plot-option 1 s m 3 Al3Sc_prim          $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_prim PHASE BOUNDARY
$*************************************************************************************
enter-composition wp sc=1                   $changes the composition, due to the error
set-temperature-celsius 1000                $defines start temperature
calculate-equilibrium                       $calculates equilibrium for set temperature
search-phase-boundary t al3sc               $defines and executes the search for the
                                            $phase boundary
set-step-option p al3sc                     $defines target phase
step-equilibrium                            $executes stepped equilibrium calculation
```

B) Script of the equilibrium phase diagram modeling with optimization of the database (Approach 1)

```
$*****************************************************************************************
$ GENERAL INFORMATION
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$Script of the modeling of the equilibrium phase diagram with optimization of the database (Approach 1)
$Database: mc_al.v2.001.tdb
$Author: René Wang
$Date of creation: 2016-10-16
$MatCalc version 5.60
$MatCalc-file name: Al-SC_eq-phase-diagram_appr_1.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t SE(AL3SC) 298,16 +400; 6000 N        $Changes the parameter SE(Al3Sc)
edit-parameter r t G(LIQUID,SC;0) 273 -5070+1*GSCLIQ#; 3200 N   $Changes the parameter G(LIQUID,SC;0)
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t wt.% Sc           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 1 a y 1 t Temperature [°C]      $defines y-axis title
set-plot-option 1 G M X Y                       $displays grid of x-axis
set-plot-option 1G M Y Y                        $displays grid of y-axis
set-plot-option 1 s n b t$c                     $define series
set-plot-option 1 s m 0 FCC_Al                  $names the series
$*****************************************************************************************
$CALCULATION OF THE Al-MATRIX BOUNDARY
$*****************************************************************************************
set-temperature-celsius 800                     $defines start temperature
set-automatic-startvalues                       $sets automatic start values
calculate-equilibrium                           $calculates equilibrium for set temperature
search-phase-boundary t fcc_a1                  $defines and executes the search for the
                                                $phase boundary
set-step-option y p                             $defines the type of the stepped
                                                $equilibrium calculation
set-step-option r 0.00005 30 l 0.05             $defines the range of the calculation, the
```

```
                                                    $increment and the interval type
set-step-option e sc                                $defines the varying element
set-step-option p fcc_a1                            $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
set-plot-option 1 s d 0                             $locks and duplicates fcc_a1
set-plot-option 1 s m 1 Liquid                      $Renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE LIQUID PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                         $defines start temperature
calculate-equilibrium                               $calculates equilibrium for set temperature
search-phase-boundary t liquid                      $defines and executes the search for the
                                                    $phase boundary
set-step-option p liquid                            $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
set-plot-option 1 s d 1                             $locks and duplicates liquid
set-plot-option 1 s m 2 Al3Sc                       $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_sec PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                         $defines start temperature
calculate-equilibrium                               $calculates equilibrium for set temperature
search-phase-boundary t al3sc                       $defines and executes the search for the
                                                    $phase boundary
set-step-option p al3sc                             $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
```

C) Script of the equilibrium phase diagram modeling with optimization of the database (Approach 2)

```
$************************************************************************************
$ GENERAL INFORMATION
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$Script of the modeling of the equilibrium phase diagram with optimization of the database (Approach 2)
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$Date of creation: 2016-10-16
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select-elements Al Sc Va                               $selects the elements
select-phases fcc_a1 liq al3sc                         $phase selection
read-thermodyn-database                                $reads thermodynamic database
enter-composition wp sc=0.05                           $defines the alloy-system
$************************************************************************************
$OPTIMIZING PARAMETERS
$************************************************************************************
edit-parameter r t SE(AL3SC) 298,16 +400; 6000 N       $Changes the parameter SE(Al3Sc)
edit-parameter r t G(LIQUID,SC;0) 273 -5070+*GSCLIQ#; 3200 N   $Changes the parameter G(LIQUID,SC;0)
edit-parameter r t G(AL3SC,AL:SC;0) 273 -168000+14,75*T+3*GHSERAL#+1,05*GHSERSC#; 6000 N
                                                       $Changes the parameter G(LIQUID,AL,SC;0)
$************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$************************************************************************************
new-gui-window p1                                      $creates new GUI-window
set-gui-window-property 3 x stepvalue                  $define values for the default x-axis
set-gui-window-property 3 s u y                        $defines default x-axis
set-gui-window-property 3 s t wt.% Sc                  $defines title of default x-axis
set-gui-window-property 3 s f 1                        $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                        $defines position of the legend
set-gui-window-property 3 s s auto                     $defines scaling expression
set-plot-option 1 a y 1 t Temperature [°C]             $defines y-axis title
set-plot-option 1 G M X Y                              $displays grid of x-axis
set-plot-option 1G M Y Y                               $displays grid of y-axis
set-plot-option 1 s n b t$c                            $define series
set-plot-option 1 s m 0 FCC_Al                         $names the series
$************************************************************************************
$CALCULATION OF THE Al-MATRIX BOUNDARY
$************************************************************************************
set-temperature-celsius 800                            $defines start temperature
set-automatic-startvalues                              $sets automatic start values
calculate-equilibrium                                  $calculates equilibrium for set temperature
search-phase-boundary t fcc_a1                         $defines and executes the search for the
```

```
                                                    $phase boundary
set-step-option y p                                 $defines the type of the stepped
                                                    $equilibrium calculation
set-step-option r 0.00005 30 l 0.05                 $defines the range of the calculation, the
                                                    $increment and the interval type
set-step-option e sc                                $defines the varying element
set-step-option p fcc_a1                            $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
set-plot-option 1 s d 0                             $locks and duplicates fcc_a1
set-plot-option 1 s m 1 Liquid                      $Renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE LIQUID PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                         $defines start temperature
calculate-equilibrium                               $calculates equilibrium for set temperature
search-phase-boundary t liquid                      $defines and executes the search for the
                                                    $phase boundary
set-step-option p liquid                            $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
set-plot-option 1 s d 1                             $locks and duplicates liquid
set-plot-option 1 s m 2 Al3Sc                       $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_sec PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                         $defines start temperature
calculate-equilibrium                               $calculates equilibrium for set temperature
search-phase-boundary t al3sc                       $defines and executes the search for the
                                                    $phase boundary
set-step-option p al3sc                             $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
```

D) Script of the equilibrium phase diagram modeling with optimization of the database (Approach 3)

```
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$Author: René Wang
$Date of creation: 2016-10-17
$MatCalc version 5.60
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$SETUP INFORMATION
$*****************************************************************************************
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open-thermodyn-database mc_al_v2.001.tdb               $opens thermodynamic database
select-elements Al Sc Va                               $selects the elements
select-phases fcc_a1 liq al3sc                         $phase selection
read-thermodyn-database                                $reads thermodynamic database
enter-composition wp sc=0.05                           $defines the alloy-system
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t SE(AL3SC) 298,16 +800; 6000 N       $Changes the parameter SE(Al3Sc)
edit-parameter r t G(LIQUID,SC;0) 273 -5070+1*GSCLIQ#; 3200 N    $Changes the parameter G(LIQUID,SC;0)
edit-parameter r t G(AL3SC,AL:SC;0) 273 -168000+14,75*T+3*GHSERAL#+1,05*GHSERSC#; 6000 N
                                                       $Changes the parameter G(LIQUID,AL,SC;0)
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                      $creates new GUI-window
set-gui-window-property 3 x stepvalue                  $define values for the default x-axis
set-gui-window-property 3 s u y                        $defines default x-axis
set-gui-window-property 3 s t wt.% Sc                  $defines title of default x-axis
set-gui-window-property 3 s f 1                        $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                        $defines position of the legend
set-gui-window-property 3 s s auto                     $defines scaling expression
set-plot-option 1 a y 1 t Temperature [°C]             $defines y-axis title
set-plot-option 1 G M X Y                              $displays grid of x-axis
set-plot-option 1G M Y Y                               $displays grid of y-axis
set-plot-option 1 s n b t$c                            $define series
set-plot-option 1 s m 0 FCC_Al                         $names the series
$*****************************************************************************************
$CALCULATION OF THE Al-MATRIX BOUNDARY
$*****************************************************************************************
set-temperature-celsius 800                            $defines start temperature
set-automatic-startvalues                              $sets automatic start values
calculate-equilibrium                                  $calculates equilibrium for set temperature
search-phase-boundary t fcc_a1                         $defines and executes the search for the
```

```
                                                    $phase boundary
set-step-option y p                                 $defines the type of the stepped
                                                    $equilibrium calculation
set-step-option r 0.00005 30 l 0.05                 $defines the range of the calculation, the
                                                    $increment and the interval type
set-step-option e sc                                $defines the varying element
set-step-option p fcc_a1                            $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
set-plot-option 1 s d 0                             $locks and duplicates fcc_a1
set-plot-option 1 s m 1 Liquid                      $Renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE LIQUID PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                         $defines start temperature
calculate-equilibrium                               $calculates equilibrium for set temperature
search-phase-boundary t liquid                      $defines and executes the search for the
                                                    $phase boundary
set-step-option p liquid                            $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
set-plot-option 1 s d 1                             $locks and duplicates liquid
set-plot-option 1 s m 2 Al3Sc                       $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_sec PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                         $defines start temperature
calculate-equilibrium                               $calculates equilibrium for set temperature
search-phase-boundary t al3sc                       $defines and executes the search for the
                                                    $phase boundary
set-step-option p al3sc                             $defines target phase
step-equilibrium                                    $executes stepped equilibrium calculation
```

E) Script of the equilibrium phase diagram modeling with optimization of the database (Approach 4)

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the modeling of the equilibrium phase diagram with optimization of the database (Approach 4)
$Database: mc_al.v2.001.tdb
$Author: René Wang
$Date of creation: 2016-10-17
$MatCalc version 5.60
$MatCalc-file name: Al-SC_eq-phase-diagram_appr_4.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                                    $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb                         $opens thermodynamic database
select-elements Al Sc Va                                         $selects the elements
select-phases fcc_a1 liq al3sc                                   $phase selection
read-thermodyn-database                                          $reads thermodynamic database
enter-composition wp sc=0.05                                     $defines the alloy-system
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t SE(AL3SC) 298,16 +400; 6000 N                 $Changes the parameter SE(Al3Sc)
edit-parameter r t G(LIQUID,SC;0) 273 -5070+1,06*GSCLIQ#; 3200 N
                                                                 $Changes the parameter G(LIQUID,SC;0)
edit-parameter r t G(AL3SC,AL:SC;0) 273 -168000+14,75*T+3*GHSERAL#+1,05*GHSERSC#; 6000 N
                                                                 $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,SC:VA;0) 273 +1,05*GSCFCC#; 3600 N   $Changes the parameter
                                                                 $G(FCC_A1,SC:VA;0)
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                $creates new GUI-window
set-gui-window-property 3 x stepvalue                            $define values for the default x-axis
set-gui-window-property 3 s u y                                  $defines default x-axis
set-gui-window-property 3 s t wt.% Sc                            $defines title of default x-axis
set-gui-window-property 3 s f 1                                  $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                  $defines position of the legend
set-gui-window-property 3 s s auto                               $defines scaling expression
set-plot-option 1 a y 1 t Temperature [°C]                       $defines y-axis title
set-plot-option 1 G M X Y                                        $displays grid of x-axis
set-plot-option 1G M Y Y                                         $displays grid of y-axis
set-plot-option 1 s n b t$c                                      $define series
set-plot-option 1 s m 0 FCC_Al                                   $names the series
$*****************************************************************************************
$CALCULATION OF THE Al-MATRIX BOUNDARY
$*****************************************************************************************
set-temperature-celsius 800                                      $defines start temperature
```

```
set-automatic-startvalues                    $sets automatic start values
calculate-equilibrium                        $calculates equilibrium for set temperature
search-phase-boundary t fcc_a1               $defines and executes the search for the
                                             $phase boundary
set-step-option y p                          $defines the type of the stepped
                                             $equilibrium calculation
set-step-option r 0.00005 30 l 0.05          $defines the range of the calculation, the
                                             $increment and the interval type
set-step-option e sc                         $defines the varying element
set-step-option p fcc_a1                     $defines target phase
step-equilibrium                             $executes stepped equilibrium calculation
set-plot-option 1 s d 0                      $locks and duplicates fcc_a1
set-plot-option 1 s m 1 Liquid               $Renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE LIQUID PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                  $defines start temperature
calculate-equilibrium                        $calculates equilibrium for set temperature
search-phase-boundary t liquid               $defines and executes the search for the
                                             $phase boundary
set-step-option p liquid                     $defines target phase
step-equilibrium                             $executes stepped equilibrium calculation
set-plot-option 1 s d 1                      $locks and duplicates liquid
set-plot-option 1 s m 2 Al3Sc                $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_sec PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                  $defines start temperature
calculate-equilibrium                        $calculates equilibrium for set temperature
search-phase-boundary t al3sc                $defines and executes the search for the
                                             $phase boundary
set-step-option p al3sc                      $defines target phase
step-equilibrium                             $executes stepped equilibrium calculation
```

F) Script of the equilibrium phase diagram modeling with optimization of the database (Permitted Approach)

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the modeling of the equilibrium phase diagram with optimization of the database (Permitted
$Approach)
$Database: mc_al.v2.001.tdb
$Author: René Wang
$Date of creation: 2016-10-24
$MatCalc version 5.60
$MatCalc-file name: Al-Sc_eq-phase-diagram_optimized.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t wt.% Sc           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 1 a y 1 t Temperature [°C]      $defines y-axis title
set-plot-option 1 G M X Y                       $displays grid of x-axis
set-plot-option 1G M Y Y                        $displays grid of y-axis
set-plot-option 1 s n b t$c                     $define series
set-plot-option 1 s m 0 FCC_Al                  $names the series
$*****************************************************************************************
$CALCULATION OF THE Al-MATRIX BOUNDARY
$*****************************************************************************************
set-temperature-celsius 800                     $defines start temperature
set-automatic-startvalues                       $sets automatic start values
calculate-equilibrium                           $calculates equilibrium for set temperature
search-phase-boundary t fcc_a1                  $defines and executes the search for the
                                                $phase boundary
```

```
set-step-option y p                          $defines the type of the stepped
                                             $equilibrium calculation
set-step-option r 0.00005 30 l 0.05          $defines the range of the calculation, the
                                             $increment and the interval type
set-step-option e sc                         $defines the varying element
set-step-option p fcc_a1                     $defines target phase
step-equilibrium                             $executes stepped equilibrium calculation
set-plot-option 1 s d 0                      $locks and duplicates fcc_a1
set-plot-option 1 s m 1 Liquid               $Renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE LIQUID PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                  $defines start temperature
calculate-equilibrium                        $calculates equilibrium for set temperature
search-phase-boundary t liquid               $defines and executes the search for the
                                             $phase boundary
set-step-option p liquid                     $defines target phase
step-equilibrium                             $executes stepped equilibrium calculation
set-plot-option 1 s d 1                      $locks and duplicates liquid
set-plot-option 1 s m 2 Al3Sc                $renames the duplicated series
$*************************************************************************************
$CALCULATION OF THE Al3Sc_sec PHASE BOUNDARY
$*************************************************************************************
set-temperature-celsius 300                  $defines start temperature
calculate-equilibrium                        $calculates equilibrium for set temperature
search-phase-boundary t al3sc                $defines and executes the search for the
                                             $phase boundary
set-step-option p al3sc                      $defines target phase
step-equilibrium                             $executes stepped equilibrium calculation
```

G) Script of the precipitation kinetic simulation according to calculation "Marquis_4"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Marquis_4
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Marquis_4.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment marquis_4                 $creates new heat treatment
append-ht-segment marquis_4                     $appends heat segment
edit-ht-segment marquis_4 0 s 20                $defines heat segment
edit-ht-segment marquis_4 0 3 648 5*60          $defines heat segment
edit-ht-segment marquis_4 1 3 648 24*60*60      $defines heat segment
edit-ht-segment marquis_4 2 3 20 10             $defines heat segment
edit-ht-segment marquis_4 3 3 400 5*60          $defines heat segment
edit-ht-segment marquis_4 4 3 400 120*60*60     $defines heat segment
edit-ht-segment marquis_4 5 3 20 10             $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h marquis_4 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

H) Script of the precipitation kinetic simulation according to calculation "Marquis_8"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Marquis_8
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Marquis_8.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment marquis_8                 $creates new heat treatment
append-ht-segment marquis_8                     $appends heat segment
edit-ht-segment marquis_8 0 s 20                $defines heat segment
edit-ht-segment marquis_8 0 3 648 5*60          $defines heat segment
edit-ht-segment marquis_8 1 3 648 24*60*60      $defines heat segment
edit-ht-segment marquis_8 2 3 20 10             $defines heat segment
edit-ht-segment marquis_8 3 3 450 5*60          $defines heat segment
edit-ht-segment marquis_8 4 3 450 72*60*60      $defines heat segment
edit-ht-segment marquis_8 5 3 20 10             $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h marquis_8 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

I) Script of the precipitation kinetic simulation according to calculation "Iwamura_1"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Iwamura_1
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Iwamura_1.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment iwamura_1                 $creates new heat treatment
append-ht-segment iwamura_1                     $appends heat segment
edit-ht-segment iwamura_1 0 s 20                $defines heat segment
edit-ht-segment iwamura_1 0 3 913-273 60*5      $defines heat segment
edit-ht-segment iwamura_1 1 3 913-273 2*60*60   $defines heat segment
edit-ht-segment iwamura_1 2 3 0 10              $defines heat segment
edit-ht-segment iwamura_1 3 3 673-273 5*60      $defines heat segment
edit-ht-segment iwamura_1 4 3 673-273 1e6       $defines heat segment
edit-ht-segment iwamura_1 5 3 20 10             $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h iwamura_1 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

J) Script of the precipitation kinetic simulation according to calculation "Iwamura_4"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Iwamura_4
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Iwamura_4.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment iwamura_4                 $creates new heat treatment
append-ht-segment iwamura_4                     $appends heat segment
edit-ht-segment iwamura_4 0 s 20                $defines heat segment
edit-ht-segment iwamura_4 0 3 913-273 60*5      $defines heat segment
edit-ht-segment iwamura_4 1 3 913-273 2*60*60   $defines heat segment
edit-ht-segment iwamura_4 2 3 0 10              $defines heat segment
edit-ht-segment iwamura_4 3 3 913-273 5*60      $defines heat segment
edit-ht-segment iwamura_4 4 3 913-273 1e6       $defines heat segment
edit-ht-segment iwamura_4 5 3 20 10             $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h iwamura_4 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

K) Script of the precipitation kinetic simulation according to calculation "Robson_2"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Robson_2
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Robson_2.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment robson_2                  $creates new heat treatment
append-ht-segment robson_2                      $appends heat segment
edit-ht-segment robson_2 0 s 20                 $defines heat segment
edit-ht-segment robson_2 0 3 640 5*60           $defines heat segment
edit-ht-segment robson_2 1 3 640 72*60*60       $defines heat segment
edit-ht-segment robson_2 2 3 20 10              $defines heat segment
edit-ht-segment robson_2 3 3 450 5*60           $defines heat segment
edit-ht-segment robson_2 4 3 450 60*60          $defines heat segment
edit-ht-segment robson_2 5 3 20 10              $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h robson_2 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

L) Script of the precipitation kinetic simulation according to calculation "Robson_3"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Robson_3
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Robson_3.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment robson_3                  $creates new heat treatment
append-ht-segment robson_3                      $appends heat segment
edit-ht-segment robson_3 0 s 20                 $defines heat segment
edit-ht-segment robson_3 0 3 640 5*60           $defines heat segment
edit-ht-segment robson_3 1 3 640 72*60*60       $defines heat segment
edit-ht-segment robson_3 2 3 20 10              $defines heat segment
edit-ht-segment robson_3 3 3 500 5*60           $defines heat segment
edit-ht-segment robson_3 4 3 500 60*60          $defines heat segment
edit-ht-segment robson_3 5 3 20 10              $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h robson_3 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

M) Script of the precipitation kinetic simulation according to calculation "Royset_1"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Royset_1
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Royset_1.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment royset_1                  $creates new heat treatment
append-ht-segment royset_1                      $appends heat segment
edit-ht-segment royset_1 0 s 20                 $defines heat segment
edit-ht-segment royset_1 0 3 600 5*60           $defines heat segment
edit-ht-segment royset_1 1 3 600 60*60          $defines heat segment
edit-ht-segment royset_1 2 3 20 10              $defines heat segment
edit-ht-segment royset_1 3 3 230 5*60           $defines heat segment
edit-ht-segment royset_1 4 3 230 170*60*60      $defines heat segment
edit-ht-segment royset_1 5 3 20 10              $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h royset_1 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

N) Script of the precipitation kinetic simulation according to calculation "Royset_2"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Royset_2
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Royset_2.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment royset_2                  $creates new heat treatment
append-ht-segment royset_2                      $appends heat segment
edit-ht-segment royset_2 0 s 20                 $defines heat segment
edit-ht-segment royset_2 0 3 600 5*60           $defines heat segment
edit-ht-segment royset_2 1 3 600 60*60          $defines heat segment
edit-ht-segment royset_2 2 3 20 10              $defines heat segment
edit-ht-segment royset_2 3 3 270 5*60           $defines heat segment
edit-ht-segment royset_2 4 3 270 170*60*60      $defines heat segment
edit-ht-segment royset_2 5 3 20 10              $defines heat segment
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
```

```
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h royset_2 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

O) Script of the precipitation kinetic simulation according to calculation "Robson_5"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Robson_5
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Robson_5.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]    $defines y-axis title
set-plot-option 1 G M X Y                       $displays grid of x-axis
set-plot-option 1G M Y Y                        $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0              $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction    $names the series
```

```
create-new-plot X 3                                                    $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                        $defines y-axis title
set-plot-option 2 G M X Y                                              $displays grid of x-axis
set-plot-option 2 G M Y Y                                              $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                              $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                           $names the series
set-plot-option 2 A Y 1 Y log                                          $defines logarithmic y-axis
create-new-plot X 3                                                    $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                        $defines y-axis title
set-plot-option 3 G M X Y                                              $displays grid of x-axis
set-plot-option 3 G M Y Y                                              $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                                $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                    $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                                 $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                     $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                                 $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                     $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)    $names the series
set-plot-option 3 A Y 1 Y log                                          $defines logarithmic y-axis
$*************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*************************************************************************************
set-simulation-parameter c n b 1,05                                    $defines convergence control
set-simulation-parameter e 1,1e6                                       $defines simulation end time
set-simulation-parameter u 1000                                        $defines output frequency
set-simulation-parameter t I 343                                       $defines isothermal treatment
start-precipitate-simulation                                           $starts simulation
```

P) Script of the sensitivity analysis regarding the activation energy

```
$************************************************************************************************
$ GENERAL INFORMATION
$************************************************************************************************
$Script of the sensitivity analysis regarding the activation energy
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-12-15
$MatCalc version 5.60
$MatCalc-file name: prec-kin_sensitivity-analysis_Q.mcw
$************************************************************************************************
$SETUP INFORMATION
$************************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$************************************************************************************************
$OPTIMIZING PARAMETERS
$************************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$************************************************************************************************
$DEFINITION OF PRECIPITATES
$************************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$************************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$************************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 2 a y 1 t Number density [m^-3] $defines y-axis title
set-plot-option 2 G M X Y                       $displays grid of x-axis
set-plot-option 2 G M Y Y                       $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0       $define series
set-plot-option 2 s m 0 Q=173000J/mol           $names the series
set-plot-option 2 A Y 1 Y log                   $defines logarithmic y-axis
```

```
$**********************************************************************************************
$PERFORMING THE SENSITIVITY ANALYSIS
$**********************************************************************************************
set-simulation-parameter c n b 1,05                                    $defines convergence control
set-simulation-parameter e 1,1e6                                       $defines simulation end time
set-simulation-parameter u 1000                                        $defines output frequency
set-simulation-parameter t I 343                                       $defines isothermal treatment
start-precipitate-simulation                                           $starts simulation
set-plot-option 1 s d 0                                                $locks and duplicates Q=173000J/mol
set-plot-option 1 s m 1 Q=195000J/mol                                  $Renames the duplicated series
edit-parameter r t MG(FCC_A1&SC,SC:VA;0) 273 -195000+R*T*LN(+0.000531); 6000 N
                                                                       $Changes the parameter
                                                                       $MG(FCC_A1&SC,SC:VA;0)
start-precipitate-simulation                                           $starts simulation
set-plot-option 1 s d 0                                                $locks and duplicates Q=195000J/mol
set-plot-option 1 s m 1 Q=200000J/mol                                  $Renames the duplicated series
edit-parameter r t MG(FCC_A1&SC,SC:VA;0) 273 -200000+R*T*LN(+0.000531); 6000 N
                                                                       $Changes the parameter
start-precipitate-simulation                                           $starts simulation
```

Q) Script of the sensitivity analysis regarding the diffusion pre-exponential factor

```
$****************************************************************************************
$ GENERAL INFORMATION
$****************************************************************************************
$Script of the sensitivity analysis regarding the diffusion pre-exponential factor
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-12-15
$MatCalc version 5.60
$MatCalc-file name: prec-kin_sensitivity-analysis_ difprexfact.mcw
$****************************************************************************************
$SETUP INFORMATION
$****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$****************************************************************************************
$OPTIMIZING PARAMETERS
$****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$****************************************************************************************
$DEFINITION OF PRECIPITATES
$****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 2 a y 1 t Number density [m^-3] $defines y-axis title
set-plot-option 2 G M X Y                       $displays grid of x-axis
set-plot-option 2 G M Y Y                       $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0       $define series
set-plot-option 2 s m 0 D0=0,000531             $names the series
```

```
set-plot-option 2 A Y 1 Y log                                   $defines logarithmic y-axis
$*************************************************************************************
$PERFORMING THE SENSITIVITY ANALYSIS
$*************************************************************************************
set-simulation-parameter c n b 1,05                             $defines convergence control
set-simulation-parameter e 1,1e6                                $defines simulation end time
set-simulation-parameter u 1000                                 $defines output frequency
set-simulation-parameter t I 343                                $defines isothermal treatment
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates D0=0,000531
set-plot-option 1 s m 1 D0=0,001                                $Renames the duplicated series
edit-parameter r t MG(FCC_A1&SC,SC:VA;0) 273 -195000+R*T*LN(+0.001); 6000 N
                                                                $Changes the parameter
                                                                $MG(FCC_A1&SC,SC:VA;0)
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates D0=0,001
set-plot-option 1 s m 1 D0=0,1                                  $Renames the duplicated series
edit-parameter r t MG(FCC_A1&SC,SC:VA;0) 273 -200000+R*T*LN(+0.1); 6000 N
                                                                $Changes the parameter
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates D0=0,1
set-plot-option 1 s m 1 D0=1                                    $Renames the duplicated series
edit-parameter r t MG(FCC_A1&SC,SC:VA;0) 273 -200000+R*T*LN(+1); 6000 N
                                                                $Changes the parameter
start-precipitate-simulation                                    $starts simulation
```

R) Script of the sensitivity analysis regarding the incubation time constant

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the sensitivity analysis regarding the incubation time constant
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-12-15
$MatCalc version 5.60
$MatCalc-file name: prec-kin_sensitivity-analysis_inc.-time-const.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 2 a y 1 t Number density [m^-3] $defines y-axis title
set-plot-option 2 G M X Y                       $displays grid of x-axis
set-plot-option 2 G M Y Y                       $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0       $define series
set-plot-option 2 s m 0 Incub.-time-const= 1,0  $names the series
```

```
set-plot-option 2 A Y 1 Y log                                   $defines logarithmic y-axis
$*****************************************************************************************
$PERFORMING THE SENSITIVITY ANALYSIS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                             $defines convergence control
set-simulation-parameter e 1,1e6                                $defines simulation end time
set-simulation-parameter u 1000                                 $defines output frequency
set-simulation-parameter t I 343                                $defines isothermal treatment
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates Inact.-radius-factor=
                                                                $1,0
set-plot-option 1 s m 1 Incub.-time-const= 2,0                  $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 2,0                    $Changes the parameter
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates Incub.-time-const=
                                                                $2,0
set-plot-option 1 s m 1 Incub.-time-const= 0,5                  $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 0,5                    $Changes the parameter
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates Incub.-time-const=
                                                                $0,5
set-plot-option 1 s m 1 Incub.-time-const= 200                  $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 200                    $Changes the parameter
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates Incub.-time-const=
                                                                $200
set-plot-option 1 s m 1 Incub.-time-const= 300                  $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 300                    $Changes the parameter
start-precipitate-simulation                                    $starts simulation
set-plot-option 1 s d 0                                         $locks and duplicates Incub.-time-const=
                                                                $300
set-plot-option 1 s m 1 Incub.-time-const= 350                  $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 350                    $Changes the parameter
start-precipitate-simulation                                    $starts simulation
```

S) Script of the sensitivity analysis regarding the nucleation constant

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the sensitivity analysis regarding  the nucleation constant
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-12-15
$MatCalc version 5.60
$MatCalc-file name: prec-kin_sensitivity-analysis_nucl-const.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 2 a y 1 t Number density [m^-3] $defines y-axis title
set-plot-option 2 G M X Y                       $displays grid of x-axis
set-plot-option 2 G M Y Y                       $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0       $define series
set-plot-option 2 s m 0 Nucl.-const.= 1,0       $names the series
set-plot-option 2 A Y 1 Y log                   $defines logarithmic y-axis
```

```
$*****************************************************************************************
$PERFORMING THE SENSITIVITY ANALYSIS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                          $defines convergence control
set-simulation-parameter e 1,1e6                             $defines simulation end time
set-simulation-parameter u 1000                              $defines output frequency
set-simulation-parameter t I 343                             $defines isothermal treatment
start-precipitate-simulation                                 $starts simulation
set-plot-option 1 s d 0                                      $locks and duplicates Nucl.-const.=1,0
set-plot-option 1 s m 1 Nucl.-const.= 0,000125               $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N U 0,000125            $Changes the parameter
start-precipitate-simulation                                 $starts simulation
set-plot-option 1 s d 0                                      $locks and duplicates Nucl.-const.=
                                                             $0,000125
set-plot-option 1 s m 1 Nucl.-const.= 0,1                    $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N U 0,1                 $Changes the parameter
start-precipitate-simulation                                 $starts simulation
set-plot-option 1 s d 0                                      $locks and duplicates Nucl.-const.=0,1
set-plot-option 1 s m 1 Nucl.-const.= 0,01                   $Renames the duplicated series
SET_PRECIPITATION_PARAMETER al3sc_p0 N U 0,01                $Changes the parameter
start-precipitate-simulation                                 $starts simulation
```

T) Script of the sensitivity analysis regarding the inactive radius factor

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the sensitivity analysis regarding the inactive radius factor
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-12-15
$MatCalc version 5.60
$MatCalc-file name: prec-kin_sensitivity-analysis_inact.-radius-fact.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 2 a y 1 t Number density [m^-3] $defines y-axis title
set-plot-option 2 G M X Y                       $displays grid of x-axis
set-plot-option 2 G M Y Y                       $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0       $define series
set-plot-option 2 s m 0 Inact.-radius-factor= 5  $names the series
set-plot-option 2 A Y 1 Y log                   $defines logarithmic y-axis
```

```
$*****************************************************************************************
$PERFORMING THE SENSITIVITY ANALYSIS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                    $defines convergence control
set-simulation-parameter e 1,1e6                       $defines simulation end time
set-simulation-parameter u 1000                        $defines output frequency
set-simulation-parameter t I 343                       $defines isothermal treatment
start-precipitate-simulation                           $starts simulation
set-plot-option 1 s d 0                                $locks and duplicates Inact.-radius-factor=
                                                       $5
set-plot-option 1 s m 1 Inact.-radius-factor= 1        $Renames the duplicated series
set-precipitation-parameter al3sc_p0 S N Y 1 0.5e-9    $Changes the parameter
start-precipitate-simulation                           $starts simulation
set-plot-option 1 s d 0                                $locks and duplicates Inact.-radius-factor=
                                                       $1
set-plot-option 1 s m 1 Inact.-radius-factor= 10       $Renames the duplicated series
set-precipitation-parameter al3sc_p0 S N Y 10 0.5e-9   $Changes the parameter
start-precipitate-simulation                           $starts simulation
set-plot-option 1 s d 0                                $locks and duplicates Inact.-radius-factor=
                                                       $10
set-plot-option 1 s m 1 Inact.-radius-factor= 50       $Renames the duplicated series
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
start-precipitate-simulation                           $starts simulation
set-plot-option 1 s d 0                                $locks and duplicates Inact.-radius-factor=
                                                       $50
set-plot-option 1 s m 1 Inact.-radius-factor= 100      $Renames the duplicated series
set-precipitation-parameter al3sc_p0 S N Y 100 0.5e-9  $Changes the parameter
start-precipitate-simulation                           $starts simulation
set-plot-option 1 s d 0                                $locks and duplicates Inact.-radius-factor=
                                                       $100
set-plot-option 1 s m 1 Inact.-radius-factor= 500      $Renames the duplicated series
set-precipitation-parameter al3sc_p0 S N Y 500 0.5e-9  $Changes the parameter
start-precipitate-simulation                           $starts simulation
```

U) Script of the optimized precipitation kinetic simulation according to calculation "Marquis_4"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Marquis_4
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Marquis_4.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment marquis_4                 $creates new heat treatment
append-ht-segment marquis_4                     $appends heat segment
edit-ht-segment marquis_4 0 s 20                $defines heat segment
edit-ht-segment marquis_4 0 3 648 5*60          $defines heat segment
edit-ht-segment marquis_4 1 3 648 24*60*60      $defines heat segment
edit-ht-segment marquis_4 2 3 20 10             $defines heat segment
edit-ht-segment marquis_4 3 3 400 5*60          $defines heat segment
edit-ht-segment marquis_4 4 3 400 120*60*60     $defines heat segment
edit-ht-segment marquis_4 5 3 20 10             $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h marquis_4 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

V) Script of the optimized precipitation kinetic simulation according to calculation "Marquis_8"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Marquis_8
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Marquis_8.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment marquis_8                 $creates new heat treatment
append-ht-segment marquis_8                     $appends heat segment
edit-ht-segment marquis_8 0 s 20                $defines heat segment
edit-ht-segment marquis_8 0 3 648 5*60          $defines heat segment
edit-ht-segment marquis_8 1 3 648 24*60*60      $defines heat segment
edit-ht-segment marquis_8 2 3 20 10             $defines heat segment
edit-ht-segment marquis_8 3 3 450 5*60          $defines heat segment
edit-ht-segment marquis_8 4 3 450 72*60*60      $defines heat segment
edit-ht-segment marquis_8 5 3 20 10             $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h marquis_8 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

W)Script of the optimized precipitation kinetic simulation according to calculation "Iwamura_1"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Iwamura_1
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Iwamura_1.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment iwamura_1                 $creates new heat treatment
append-ht-segment iwamura_1                     $appends heat segment
edit-ht-segment iwamura_1 0 s 20                $defines heat segment
edit-ht-segment iwamura_1 0 3 913-273 60*5      $defines heat segment
edit-ht-segment iwamura_1 1 3 913-273 2*60*60   $defines heat segment
edit-ht-segment iwamura_1 2 3 0 10              $defines heat segment
edit-ht-segment iwamura_1 3 3 673-273 5*60      $defines heat segment
edit-ht-segment iwamura_1 4 3 673-273 1e6       $defines heat segment
edit-ht-segment iwamura_1 5 3 20 10             $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h iwamura_1 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

X) Script of the optimized precipitation kinetic simulation according to calculation "Iwamura_4"

```
$**********************************************************************************************
$ GENERAL INFORMATION
$**********************************************************************************************
$Script of the precipitation kinetic simulation according to Iwamura_4
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Iwamura_4.mcw
$**********************************************************************************************
$SETUP INFORMATION
$**********************************************************************************************
new-workspace                                          $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb               $opens thermodynamic database
select-elements Al Sc Va                               $selects the elements
select-phases fcc_a1 liq al3sc                         $phase selection
read-thermodyn-database                                $reads thermodynamic database
enter-composition wp sc=0.05                           $defines the alloy-system
read-mobility-database                                 $reads diffusion database
$**********************************************************************************************
$OPTIMIZING PARAMETERS
$**********************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$**********************************************************************************************
$DEFINITION OF PRECIPITATES
$**********************************************************************************************
create-precipitation-domain matrix                     $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1            $defines the domain
create-new-phase al3sc p                               $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b             $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25              $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500           $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$**********************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$**********************************************************************************************
create-heat-treatment iwamura_4                        $creates new heat treatment
append-ht-segment iwamura_4                            $appends heat segment
edit-ht-segment iwamura_4 0 s 20                       $defines heat segment
edit-ht-segment iwamura_4 0 3 913-273 60*5             $defines heat segment
edit-ht-segment iwamura_4 1 3 913-273 2*60*60          $defines heat segment
edit-ht-segment iwamura_4 2 3 0 10                     $defines heat segment
edit-ht-segment iwamura_4 3 3 913-273 5*60             $defines heat segment
edit-ht-segment iwamura_4 4 3 913-273 1e6              $defines heat segment
edit-ht-segment iwamura_4 5 3 20 10                    $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h iwamura_4 10                            $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

Y) Script of the optimized precipitation kinetic simulation according to calculation "Robson_2"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Robson_2
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Robson_2.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment robson_2                  $creates new heat treatment
append-ht-segment robson_2                      $appends heat segment
edit-ht-segment robson_2 0 s 20                 $defines heat segment
edit-ht-segment robson_2 0 3 640 5*60           $defines heat segment
edit-ht-segment robson_2 1 3 640 72*60*60       $defines heat segment
edit-ht-segment robson_2 2 3 20 10              $defines heat segment
edit-ht-segment robson_2 3 3 450 5*60           $defines heat segment
edit-ht-segment robson_2 4 3 450 60*60          $defines heat segment
edit-ht-segment robson_2 5 3 20 10              $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h robson_2 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

Z) Script of the optimizes precipitation kinetic simulation according to calculation "Robson_3"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Robson_3
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Robson_3.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment robson_3                  $creates new heat treatment
append-ht-segment robson_3                      $appends heat segment
edit-ht-segment robson_3 0 s 20                 $defines heat segment
edit-ht-segment robson_3 0 3 640 5*60           $defines heat segment
edit-ht-segment robson_3 1 3 640 72*60*60       $defines heat segment
edit-ht-segment robson_3 2 3 20 10              $defines heat segment
edit-ht-segment robson_3 3 3 500 5*60           $defines heat segment
edit-ht-segment robson_3 4 3 500 60*60          $defines heat segment
edit-ht-segment robson_3 5 3 20 10              $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h robson_3 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

AA) Script of the optimized precipitation kinetic simulation according to calculation "Royset_1"

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Royset_1
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Royset_1.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$*****************************************************************************************
create-heat-treatment royset_1                  $creates new heat treatment
append-ht-segment royset_1                      $appends heat segment
edit-ht-segment royset_1 0 s 20                 $defines heat segment
edit-ht-segment royset_1 0 3 600 5*60           $defines heat segment
edit-ht-segment royset_1 1 3 600 60*60          $defines heat segment
edit-ht-segment royset_1 2 3 20 10              $defines heat segment
edit-ht-segment royset_1 3 3 230 5*60           $defines heat segment
edit-ht-segment royset_1 4 3 230 170*60*60      $defines heat segment
edit-ht-segment royset_1 5 3 20 10              $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h royset_1 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

BB) Script of the optimized precipitation kinetic simulation according to calculation "Royset_2"

```
$************************************************************************************
$ GENERAL INFORMATION
$************************************************************************************
$Script of the precipitation kinetic simulation according to Royset_2
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Royset_2.mcw
$************************************************************************************
$SETUP INFORMATION
$************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$************************************************************************************
$OPTIMIZING PARAMETERS
$************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$************************************************************************************
$DEFINITION OF PRECIPITATES
$************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$************************************************************************************
$DEFINITION OF THE HEAT TREATMENT
$************************************************************************************
create-heat-treatment royset_2                  $creates new heat treatment
append-ht-segment royset_2                      $appends heat segment
edit-ht-segment royset_2 0 s 20                 $defines heat segment
edit-ht-segment royset_2 0 3 600 5*60           $defines heat segment
edit-ht-segment royset_2 1 3 600 60*60          $defines heat segment
edit-ht-segment royset_2 2 3 20 10              $defines heat segment
edit-ht-segment royset_2 3 3 270 5*60           $defines heat segment
edit-ht-segment royset_2 4 3 270 170*60*60      $defines heat segment
edit-ht-segment royset_2 5 3 20 10              $defines heat segment
```

```
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                                                    $creates new GUI-window
set-gui-window-property 3 x stepvalue                                $define values for the default x-axis
set-gui-window-property 3 s u y                                      $defines default x-axis
set-gui-window-property 3 s t Time[h]                                $defines title of default x-axis
set-gui-window-property 3 s f 1                                      $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                                      $defines position of the legend
set-gui-window-property 3 s s auto                                   $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]                         $defines y-axis title
set-plot-option 1 G M X Y                                            $displays grid of x-axis
set-plot-option 1G M Y Y                                             $displays grid of y-axis
set-plot-option 1 s n b F$AL3SC_P0                                   $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                         $names the series
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                      $defines y-axis title
set-plot-option 2 G M X Y                                            $displays grid of x-axis
set-plot-option 2 G M Y Y                                            $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                            $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                         $names the series
set-plot-option 2 A Y 1 Y log                                        $defines logarithmic y-axis
create-new-plot X 3                                                  $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                      $defines y-axis title
set-plot-option 3 G M X Y                                            $displays grid of x-axis
set-plot-option 3 G M Y Y                                            $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                               $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                   $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                            $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight)  $names the series
set-plot-option 3 A Y 1 Y log                                        $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                  $defines convergence control
set-simulation-parameter e 1,1e6                                     $defines simulation end time
set-simulation-parameter u 1000                                      $defines output frequency
set-simulation-parameter t h royset_2 10                             $chooses heat treatment
start-precipitate-simulation                                         $starts simulation
```

CC) Script of the optimizes precipitation kinetic simulation according to calculation “Robson_5”

```
$*****************************************************************************************
$ GENERAL INFORMATION
$*****************************************************************************************
$Script of the precipitation kinetic simulation according to Robson_5
$Databases: mc_al.v2.001.tdb, mc_al.v2.001.ddb
$Author: René Wang
$Date of creation: 2016-11-08
$MatCalc version 5.60
$MatCalc-file name: Robson_5.mcw
$*****************************************************************************************
$SETUP INFORMATION
$*****************************************************************************************
new-workspace                                   $opens new workspace
open-thermodyn-database mc_al_v2.001.tdb        $opens thermodynamic database
select-elements Al Sc Va                        $selects the elements
select-phases fcc_a1 liq al3sc                  $phase selection
read-thermodyn-database                         $reads thermodynamic database
enter-composition wp sc=0.05                    $defines the alloy-system
read-mobility-database                          $reads diffusion database
$*****************************************************************************************
$OPTIMIZING PARAMETERS
$*****************************************************************************************
edit-parameter r t G(LIQUID,AL,SC;0) 273 -163000+10*T; 6000 N   $Changes the parameter G(LIQUID,AL,SC;0)
edit-parameter r t G(FCC_A1,AL,SC:VA;0) 273 -112376; 6000 N     $Changes the parameter
                                                                $G(FCC_A1,AL,SC:VA;0)
edit-parameter r t G(LIQUID,AL,SC;1) 273 +21300; 6000 N         $Changes the parameter G(LIQUID,AL,SC;1)
$*****************************************************************************************
$DEFINITION OF PRECIPITATES
$*****************************************************************************************
create-precipitation-domain matrix              $creates precipitation domain
set-precipitation-parameter matrix x fcc_a1     $defines the domain
create-new-phase al3sc p                        $creates the precipitate phase
set-precipitation-parameter al3sc_p0 n s b      $defines homogeneous precipitation
set-precipitation-parameter al3sc_p0 c 25       $defines number of size classes
SET_PRECIPITATION_PARAMETER al3sc_p0 N T 500    $Changes the incubation time constant
set-precipitation-parameter al3sc_p0 S N Y 50 0.5e-9   $Changes the parameter
$*****************************************************************************************
$SETTING UP THE OUTPUT WINDOW
$*****************************************************************************************
new-gui-window p1                               $creates new GUI-window
set-gui-window-property 3 x stepvalue           $define values for the default x-axis
set-gui-window-property 3 s u y                 $defines default x-axis
set-gui-window-property 3 s t Time[h]           $defines title of default x-axis
set-gui-window-property 3 s f 1                 $defines scaling factor of default x-axis
set-gui-window-property 3 s l b                 $defines position of the legend
set-gui-window-property 3 s s auto              $defines scaling expression
set-plot-option 1 a y 1 t Phase Fraction [%]    $defines y-axis title
set-plot-option 1 G M X Y                       $displays grid of x-axis
set-plot-option 1G M Y Y                        $displays grid of y-axis
```

```
set-plot-option 1 s n b F$AL3SC_P0                                  $define series
set-plot-option 1 s m 0 Al3Sc-Phase Fraction                        $names the series
create-new-plot X 3                                                 $adds new plot to GUI-window
set-plot-option 2 a y 1 t Number density [m^-3]                     $defines y-axis title
set-plot-option 2 G M X Y                                           $displays grid of x-axis
set-plot-option 2 G M Y Y                                           $displays grid of y-axis
set-plot-option 2 s n b NUM_PREC$AL3SC_P0                           $define series
set-plot-option 2 s m 0 Al3Sc-Number Density                        $names the series
set-plot-option 2 A Y 1 Y log                                       $defines logarithmic y-axis
create-new-plot X 3                                                 $adds new plot to GUI-window
set-plot-option 3 a y 1 Precipitate Radius [nm]                     $defines y-axis title
set-plot-option 3 G M X Y                                           $displays grid of x-axis
set-plot-option 3 G M Y Y                                           $displays grid of y-axis
set-plot-option 3 s n b R_CRIT$AL3SC_P0                             $define series
set-plot-option 3 s m 0 Critical Precipitate Radius                 $names the series
set-plot-option 3 s n b R_MIN$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Minimum Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MAX$AL3SC_P0                              $define series
set-plot-option 3 s m 0 Maximum Precipitate Radius                  $names the series
set-plot-option 3 s n b R_MVMEAN$AL3SC_P0                           $define series
set-plot-option 3 s m 0 Mean Precipitate Radius (volumetric weight) $names the series
set-plot-option 3 A Y 1 Y log                                       $defines logarithmic y-axis
$*****************************************************************************************
$SIMULATION OF THE PRECIPITATION KINETICS
$*****************************************************************************************
set-simulation-parameter c n b 1,05                                 $defines convergence control
set-simulation-parameter e 1,1e6                                    $defines simulation end time
set-simulation-parameter u 1000                                     $defines output frequency
set-simulation-parameter t I 343                                    $defines isothermal treatment
start-precipitate-simulation                                        $starts simulation
```

DD) Comparison of all equilibrium phase diagram modeling approaches

Literature values [9]			Original Calculation			Approach 1			Approach 2			Approach 3			Approach 4			Permitted Approach		
Sc-concentration		Phase boundary temperature	Phase boundary temperature	Deviation		Phase boundary temperature	Deviation		Phase boundary temperature	Deviation		Phase boundary temperature	Deviation		Phase boundary temperature	Deviation		Phase boundary temperature	Deviation	
wt.%	at.%	°C	Calculated [°C]	abs. [°C]	%	Calculated [°C]	abs. [°C]	%	Calculated [°C]	abs. [°C]	%	Calculated [°C]	abs. [°C]	%	Calculated [°C]	abs. [°C]	%	Calculated [°C]	abs. [°C]	%
0,01	0,006	380,00	376,98	-3,02	-0,46	382,77	2,77	0,42	379,82	-0,18	-0,03	360,17	-19,83	-3,04	381,68	1,68	0,26	362,26	-17,74	-2,72
0,02	0,012	420,00	418,84	-1,16	-0,17	402,77	-17,23	-2,49	419,82	-0,18	-0,03	400,17	-19,83	-2,86	401,68	-18,32	-2,64	402,26	-17,74	-2,56
0,03	0,018	442,00	445,97	3,97	0,56	422,77	-19,23	-2,69	439,82	-2,18	-0,31	420,17	-21,83	-3,05	441,68	-0,32	-0,04	428,13	-13,87	-1,94
0,04	0,020	460,00	466,58	6,58	0,90	442,77	-17,23	-2,35	459,82	-0,18	-0,03	460,17	0,17	0,02	461,68	1,68	0,23	448,28	-11,72	-1,60
0,05	0,030	477,00	483,43	6,43	0,86	462,77	-14,23	-1,90	479,82	2,82	0,38	470,17	-6,83	-0,91	475,00	-2,00	-0,27	464,95	-12,05	-1,61
0,10	0,060	530,00	541,29	11,29	1,41	522,77	-7,23	-0,90	539,82	9,82	1,22	520,17	-9,83	-1,22	521,00	-9,00	-1,12	522,26	-7,74	-0,96
0,15	0,090	566,00	576,70	10,70	1,28	562,77	-3,23	-0,38	579,82	13,82	1,65	560,17	-5,83	-0,69	561,68	-4,32	-0,51	559,01	-6,99	-0,83
0,20	0,120	592,00	609,43	17,43	2,01	602,77	10,77	1,24	619,82	27,82	3,22	595,17	3,17	0,37	590,00	-2,00	-0,23	587,98	-4,02	-0,46
0,25	0,150	615,00	634,11	19,11	2,15	612,77	-2,23	-0,25	639,82	24,82	2,79	620,17	5,17	0,58	611,00	-4,00	-0,45	612,06	-2,94	-0,33
0,30	0,180	635,00	655,44	20,44	2,25	622,77	-12,23	-1,35	659,82	24,82	2,73	640,17	5,17	0,57	631,00	-4,00	-0,44	632,94	-2,06	-0,23
0,35	0,210	650,00	692,26	42,26	4,58	647,00	-3,00	-0,32	659,82	9,82	1,06	659,70	9,70	1,05	655,00	5,00	0,54	651,53	1,53	0,17
0,39	0,230	660,00	700,24	40,24	4,31	659,64	-0,36	-0,04	659,82	-0,18	-0,02	659,70	-0,30	-0,03	659,60	-0,40	-0,04	659,61	-0,39	-0,04
0,55	0,360	659,00	739,14	80,14	8,60	659,64	0,64	0,07	684,01	25,01	2,68	667,81	8,81	0,95	659,60	0,60	0,06	659,61	0,61	0,07
3,30	2,000	820,00	921,00	101,00	9,24	837,95	17,95	1,64	874,73	54,73	5,01	854,12	34,12	3,12	835,56	15,56	1,42	839,60	19,60	1,79
6,50	4,000	940,00	1014,00	74,00	6,10	926,14	-13,86	-1,14	969,65	29,65	2,44	947,61	7,61	0,63	922,24	-17,76	-1,46	929,91	-10,09	-0,83
9,60	6,000	1025,00	1077,00	52,00	4,01	986,09	-38,91	-3,00	1034,19	9,19	0,71	1011,39	-13,61	-1,05	981,08	-43,92	-3,38	991,91	-33,09	-2,55
12,70	8,000	1085,00	1128,00	43,00	3,17	1035,24	-49,76	-3,66	1087,06	2,06	0,15	1063,77	-21,23	-1,56	1029,27	-55,73	-4,10	1043,06	-41,94	-3,09
15,60	10,000	1120,00	1169,00	49,00	3,52	1075,38	-44,62	-3,20	1130,16	10,16	0,73	1106,56	-13,44	-0,97	1068,62	-51,38	-3,69	1084,97	-35,03	-2,51
18,50	12,000	1170,00	1205,00	35,00	2,43	1111,22	-58,78	-4,07	1168,59	-1,41	-0,10	1144,76	-25,24	-1,75	1103,74	-66,26	-4,59	1122,46	-47,54	-3,29
21,30	14,000	1205,00	1237,00	32,00	2,16	1142,06	-62,94	-4,26	1201,63	-3,37	-0,23	1177,64	-27,36	-1,85	1133,96	-71,04	-4,81	1154,75	-50,25	-3,40
24,10	16,000	1235,00	1264,00	29,00	1,92	1169,05	-65,95	-4,37	1230,52	-4,48	-0,30	1206,41	-28,59	-1,90	1160,41	-74,59	-4,95	1183,01	-51,99	-3,45
26,80	18,000	1260,00	1286,00	26,00	1,70	1191,00	-69,00	-4,50	1253,99	-6,01	-0,39	1229,78	-30,22	-1,97	1181,91	-78,09	-5,09	1205,99	-54,01	-3,52
29,40	20,000	1280,00	1303,00	23,00	1,48	1207,77	-72,23	-4,65	1271,91	-8,09	-0,52	1247,64	-32,36	-2,08	1198,34	-81,66	-5,26	1223,54	-56,46	-3,64

EE) Comparison of all calculations of the precipitation kinetic simulations

				Literature Data		Without Optimization					Optimized				
Reference	Shorthand Symbol	Heat Treatment	Composition	Mean Precipitate Radius [nm]	Phase Fraction	Calculated Precipitate Radius r_v_mean [nm]	r_mean Deviation absolute	r_mean Deviation [%]	Calculated Phase Fraction	Phase Fraction Deviation absolute	Phase Fraction Deviation [%]	Calculated Precipitate Radius r_v_mean [nm]	r_mean Deviation absolute	r_mean Deviation [%]	Calculated Phase Fraction	Phase Fraction Deviation absolute	Phase Fraction Deviation [%]
Marquis E.A. (2001)	Marquis_1	648°C for 24h + Quenching + 300°C for 6h + Quenching	Al-0,3 wt.% Sc	1	-	1,39	0,39	39,00	0,006800	-	-	1,65	0,65	65,00	0,006800	-	-
	Marquis_2	648°C for 24h + Quenching + 350°C for 24h + Quenching	Al-0,3 wt.% Sc	5	0,0097	4,21	-0,79	-15,80	0,006888	-0,0002802	-28,92	5,26	0,26	5,20	0,006917	-0,002773	-28,62
	Marquis_3	648°C for 24h + Quenching + 400°C for 1h + Quenching	Al-0,3 wt.% Sc	5	0,0067	4,20	-0,80	-16,00	0,006483	-0,0002577	-3,81	5,40	0,40	8,00	0,006484	-0,0002562	-3,80
	Marquis_4	648°C for 24h + Quenching + 400°C for 120h + Quenching	Al-0,3 wt.% Sc	20	0,0067	17,73	-2,27	-11,35	0,006694	-0,0000462	-0,68	22,10	2,10	10,50	0,006694	-0,0000462	-0,68
	Marquis_5	648°C for 24h + Quenching + 300°C for 72h + Quenching	Al-0,1 wt.% Sc	8,8	-	1,84	-6,96	-79,09	0,002200	-	-	5,70	-3,10	-35,23	0,002200	-	-
	Marquis_6	648°C for 24h + Quenching + 300°C for 72h + Quenching	Al-0,2 wt.% Sc	3	-	2,20	-0,80	-26,67	0,004600	-	-	4,04	1,04	34,67	0,004600	-	-
	Marquis_7	648°C for 24h + Quenching + 300°C for 72h + Quenching	Al-0,3 wt.% Sc	2	0,0071	2,23	0,23	11,50	0,007009	-0,0000051	-0,72	2,79	0,79	39,50	0,007009	-0,0000051	-0,72
	Marquis_8	648°C for 24h + Quenching + 450°C for 72h + Quenching	Al-0,3 wt.% Sc	40	0,0064	37,17	-2,83	-7,07	0,006189	-0,0002001	-3,15	45,09	5,09	12,73	0,006189	-0,0002001	-3,15
	Marquis_9	648°C for 24h + Quenching + 300°C for 120h + Quenching	Al-0,3 wt.% Sc	7	-	9,01	2,01	28,71	0,007000	-	-	11,28	4,28	61,14	0,007000	-	-
	Marquis_10	648°C for 24h + Quenching + 300°C for 350h + Quenching	Al-0,3 wt.% Sc	3	-	3,14	0,14	4,67	0,007059	-	-	3,18	0,18	6,00	0,007066	-	-
Berezina et al. (1990)	Berezina	isothermal at 300°C for 350h	Al-0,3 wt.% Sc	5	-	3,43	-1,57	-31,40	0,007100	-	-	4,60	-0,40	-8,00	0,007100	-	-
Sano et al. (1990)	Sano	isothermal at 300°C for 6x10^5s	Al-0,25 wt.% Sc	9	-	3,00	-6,00	-66,67	0,005800	-	-	4,16	-4,84	-53,78	0,005800	-	-
Miura et al. (1993)	Miura	isothermal at 350°C for 10^6s	Al-0,23 wt.% Sc	4	-	8,13	4,13	103,25	0,005300	-	-	11,15	7,15	178,75	0,005300	-	-
Novotny G. (2001)	Novotny_1	642°C for 2h + Quenching + 350°C for 72h + Quenching	Al-0,3 wt.% Sc	5	0,0069	5,50	0,50	10,00	0,006925	0,0000025	0,36	7,12	2,12	42,40	0,006925	0,0000025	0,36
	Novotny_2	642°C for 2h + Quenching + 350°C for 6month + Quenching	Al-0,2 wt.% Sc	15	0,0044	18,04	3,04	20,27	0,004640	0,0002040	5,44	23,38	8,38	55,87	0,004646	0,0002046	5,59
Iwamura S. (2004)	Iwamura_1	640°C for 2h + Quenching + 400°C for 10^6s + Quenching	Al-0,2 wt.% Sc	21	-	23,13	2,13	10,14	0,004300	-	-	28,81	7,81	37,19	0,004300	-	-
	Iwamura_2	640°C for 2h + Quenching + 430°C for 10^6s + Quenching	Al-0,2 wt.% Sc	41	-	39,72	-1,28	-3,12	0,004000	-	-	50,20	9,20	22,44	0,004000	-	-
	Iwamura_3	640°C for 2h + Quenching + 460°C for 10^6s + Quenching	Al-0,2 wt.% Sc	76	-	69,26	-6,74	-8,87	0,003700	-	-	82,95	6,95	9,14	0,003700	-	-
	Iwamura_4	640°C for 2h + Quenching + 490°C for 10^6s + Quenching	Al-0,2 wt.% Sc	121	-	107,57	-13,43	-11,10	0,003100	-	-	133,33	12,33	10,19	0,003100	-	-
Robson J.D. (2003)	Robson_1	640°C for 72h + Quenching + 400°C for 1h + Quenching	Al-0,25 wt.% Sc	3,5	-	4,94	1,44	41,14	0,005329	-	-	5,19	1,69	48,29	0,005317	-	-
	Robson_2	640°C for 72h + Quenching + 450°C for 1h + Quenching	Al-0,25 wt.% Sc	8,5	0,0046	9,22	0,72	8,47	0,004820	0,0002220	4,78	11,63	3,13	36,82	0,004861	0,0002261	5,67
	Robson_3	640°C for 72h + Quenching + 500°C for 1h + Quenching	Al-0,25 wt.% Sc	20	0,0036	20,49	0,49	2,45	0,003988	0,0003388	10,78	25,04	5,04	25,20	0,004019	0,0004419	11,64
	Robson_4	640°C for 72h + Quenching + 550°C for 1h + Quenching	Al-0,25 wt.% Sc	54	0,0023	41,14	-12,86	-23,81	0,002612	0,0003362	16,09	48,89	-5,11	-9,46	0,002634	0,0003384	17,08
	Robson_5	isothermal 343°C for 1h	Al-0,183 at.% Sc	-	-	1,56	-	-	0,003900	-	-	5,75	-	-	0,003999	-	-
Clouet E. (2006)	Clouet_1	isothermal at 300°C for 10^6s	Al-0,18 at.% Sc	2,5	-	2,98	0,48	19,20	0,007084	-	-	4,16	1,66	66,40	0,007106	-	-
	Clouet_2	isothermal at 350°C for 10^6s	Al-0,18 at.% Sc	7	-	7,47	0,47	6,71	0,007007	-	-	9,94	2,94	42,00	0,007020	-	-
	Clouet_3	isothermal at 300°C for 10^6s	Al-0,18 at.% Sc	19	-	21,03	2,03	10,68	0,006811	-	-	27,01	8,01	42,16	0,006819	-	-
Royset (2005)	Royset_1	600°C for 1h + Quenching to 230°C and holding 170h + Quenching	Al-0,2 wt.% Sc	-	0,0043	0,69	-	-	0,004353	0,0000074	1,73	0,77	-	-	0,004348	0,0000069	1,61
	Royset_2	600°C for 1h + Quenching to 270°C and holding 170h + Quenching	Al-0,2 wt.% Sc	-	0,0043	1,55	-	-	0,004561	0,0000282	6,59	2,14	-	-	0,004708	0,0000429	10,03
	Royset_3	600°C for 1h + Quenching to 330°C and holding 170h + Quenching	Al-0,2 wt.% Sc	-	0,0043	4,83	-	-	0,004597	0,0000318	7,43	6,24	-	-	0,004612	0,0000333	7,78
	Royset_4	600°C for 1h + Quenching to 370°C and holding 170h + Quenching	Al-0,2 wt.% Sc	-	0,0043	11,48	-	-	0,004470	0,0000191	4,46	13,61	-	-	0,004480	0,0000201	4,70

FF) File-directory