Bernhard Fercher, BSc

Modelling of the microstructure and creep deformation of creep resistant steel P91

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Univ.-Prof. Dipl.-Ing. Dr.techn. Bernhard Sonderegger

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AFFIDAVIT

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Abstract

Creep resistant materials are an essential part of many modern high temperature applications, ranging from precisely manufactured turbine components to just simple steam pipes in caloric power plants. The reliable prediction of the remaining service life of already installed components using creep models is of greatest scientific and economic interest. This also includes the need to accurately predict the creep behaviour of newly developed materials without having to wait for experimental creep data.

The present work is based on an existing semi-physical creep model, which was developed and optimized by the IMAT modelling group at Graz University of Technology in the course of several preceding projects and studies.

The practical realisation of the model consists of a combination of a simulation of the material's microstructural evolution using the scientific software toolbox 'MatCalc' and the implementation of the mathematical formulae in the programming environment of 'Matlab'.

The aim of this work is the further development of the model to yield more reliable and universal valid results. This is achieved by creating new MatCalc scripts to calculate phase equilibria, Scheil-Gulliver solidification simulations and precipitation kinetics simulations. For this purpose, numerous changes are made in the mathematical model itself as well as the coding of the model in Matlab.

Ultimately, this work leads to improvements in predicting material's service live even with deviating parameters for temperature and tensile stress. Various changes to the programming implementation of the model in Matlab supplement this with a more comfortable and now partially automated operation of the model. This is especially true when several data sets are used simultaneously.

The findings from this master's thesis and the generated code form a stable foundation for promising further work on this creep model.

Kurzfassung

Kriechbeständige Materialien sind ein essentieller Bestandteil von vielen modernen Hochtemperaturanwendungen, seien es präzise gefertigte Turbinenbestandteile oder nur einfache Dampfleitungen in kalorischen Kraftwerken. Die zuverlässige Vorhersage der verbleibenden Lebensdauer von bereits verbauten Komponenten mit Hilfe von Kriechmodellen ist dabei von größtem wissenschaftlichen und wirtschaftlichem Interesse. Dies umfasst auch den Wunsch zur exakten Vorhersage des Kriechverhaltens von neu entwickelten Werkstoffen, ohne auf experimentelle Kriechdaten warten zu müssen.

Die vorliegende Arbeit baut dabei auf ein bestehendes semi-physikalisches Kriechmodell auf, welches im Rahmen mehrerer Projekte und Arbeiten von der Modellierungsgruppe am IMAT an der TU Graz erstellt und optimiert wurde.

Die Umsetzung des Modells besteht dabei aus einer Kombination einer Simulation der mikrostrukturellen Entwicklung des zu simulierenden Materials mittels der Software-Toolbox 'MatCalc' und der Implementierung des mathematischen Formelwerkes in der Programmierumgebung von 'Matlab'.

Ziel dieser Arbeit ist nun die weitere Entwicklung des gesamten Modells um zuverlässigere und universeller gültige Ergebnisse liefern zu können. Dies geschieht durch die Schaffung von neuen MatCalc-Skripen zur Berechnung von Phasengleichgewichten, Scheil-Gulliver-Erstarrungssimulationen und Ausscheidungskinetiksimulationen. Dazu erfolgen zahlreiche Umstellungen am mathematischen Modell und an der programmiertechnischen Umsetzung in Matlab.

Letzendlich führt diese Arbeit zu Verbesserungen an berechneten Standzeiten auch bei abweichenden Temperatur- und Zugspannungs-Parametern. Die diversen Änderungen an der Implementierung in Matlab ergänzen dies durch eine komfortablere und nun teilautomatisierte Bedienung des Modells, vor allem bei der Verwendung mehrerer Datensätze gleichzeitig.

Die Erkenntnisse aus dieser Masterarbeit und der generierte Code bilden dabei ein stabiles Fundament für vielversprechende weitergehende Arbeiten am diesem Kriechmodell.

Variables and parameters

The first columns in tables 1 and 2 refer to the variables and constants used in this thesis. The second columns show the corresponding names used in the Matlab-code as printed in the appendix. Table 3 lists all noteworthy abbreviations used.

Table 1.: Variables and parameters part 1

symbol	Matlab	unit	description
a_1	a1	[ ]	parameter for glide velocity
a_g	ag	[m]	unit cell size
A	A	[ ]	material specific constant
α	alpha	[ ]	constant for dislocation interaction
b	b	[m]	burgers vector
β	beta	[ ]	parameter to control the density of sources
c_{dip}	c_dip	[ ]	weighting factor
d_{anh}	d_anh	[m]	dislocation annihilation length
D_{cav}	D_cav	[ ]	cavitation damage parameter
D_{ppt}	D_prc	[ ]	precipitates coarsening damage parameter
D_s	Ds	[m^2/s]	coefficient for self diffusion
D_{vp}	Dvp	[m^2/s]	coefficient for pipe diffusion
ε	strain	[%]	creep strain
$\dot{\varepsilon}$	rate_strain	[%/s]	creep strain rate
η_v	eta	[ ]	vacancies transfer coefficient
G	G	[Pa]	shear modulus
γ_{sgb}	Vsb	[J]	subgrain boundary surface energy
h_b	Hb	[m]	spacing of dislocations within subgrain walls
h_m	Hm	[m]	spacing between mobile dislocations
k_B	k	[J/K]	Boltzmann's constant
k_d	Kd	[m^3/s]	parameter for coarsening
k_p	Kp	[1/s]	another parameter for coarsening
l	l	[ ]	material specific parameter for coarsening
L_α	L_alpha_v	[m]	interaction length between dislocations and defects
L_p	Lp	[m]	diffusion path length along dislocation core
M	M	[ ]	Taylor factor
M_{sgb}	Msb	[$m/Pa \cdot s$]	Mobility of subgrain boundaries
$N_{V,initial}$	Nvpo	[$1/m^3$]	number density initial start value
N_V	Nvp	[$1/m^3$]	number density without MatCalc data
N_V	Nvp_eff	[$1/m^3$]	effective number density with MatCalc data
ν	ny	[ ]	Poisson's ratio

Table 2.: Variables and parameters part 2

symbol	Matlab	unit	description
π	Pi	[ ]	the number Pi
P_{sgb}	Ps	[Pa]	subgrain growth pressure
Q	Q	[J]	activation energy
$r_{initial}$	rpo	[m]	initial precipitates radius
r_{mean}	rp	[m]	precipitates mean radius
R_{sg}	R_sgb	[m]	subgrain mean radius
ρ_b	disdens_b	[1/m²]	boundary dislocation density
ρ_{dip}	disdens_dip	[1/m²]	dipole dislocation density
ρ_m	disdens_m	[1/m²]	mobile dislocation density
ρ_t	disdens_t	[1/m²]	total dislocation density
σ_{app}	sigma_applied	[Pa]	applied stress
σ_{app_0}	sigma_applied_c	[Pa]	applied initial stress
σ_{eff}	sigma_effective	[Pa]	effective stress
σ_i	sigma_i	[Pa]	internal stress
t	time	[s]	time
T	T	[K]	temperature
v_c	vc	[m/s]	dislocations climb velocity
v_{cc}	vc_neu	[m/s]	dislocations constant climb velocity
v_{cl}	vcl	[m/s]	lattice diffusion climb velocity
v_{cp}	vcp	[m/s]	pipe diffusion climb velocity
v_{eff}	v_eff	[m/s]	effective velocity of mobile dislocations
v_g	vg	[m/s]	dislocations glide velocity
W	W	[J]	pipe diffusion activation energy
Ω	omega	[m³]	atomic volume
Ω_{mult}	omega_mult	[ ]	dislocation movement displacement factor
ζ	zeta	[ ]	factor of influence of dislocation dipoles on boundary dislocations

Table 3.: Table of abbreviations

short	long name
ASME	American Society of Mechanical Engineers
BM	Base metal
CDM	Continuum damage mechanics
CMOS	Complementary metal-oxide-semiconductor
EBSD	Electron backscatter diffraction
ECCC	European Creep Collaborative Committee
FGHAZ	Fine grain heat-affected zone
GUI	Graphical user interface
NIMS	National Institute for Materials Science
PWHT	Post weld heat treatment
SEM	Scanning electron microscope
TEM	Transmission electron microscope
TTR	Time to rupture

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1. Introduction

The phenomenon of creep (slow permanent plastic deformation under the influence of mechanical stress and elevated temperatures) is one limiting factor for service life of thermal power plants. All pressurised parts in contact with superheated steam are especially susceptible to creep, which e.g. includes pipes and turbine components. A frequently used material for these structures is the martensitic steel X10CrMoVNb9-1, also known as 'Grade 91' alloy steel.

To achieve satisfying efficiency - which saves fuel and reduces total CO_2 emissions - the current operating conditions go as high as 600 °C and stresses of 100 MPa. It should be noted that the service life decreases exponentially with rising thermal- and pressure levels.

New materials may achieve better service times at even higher temperatures while maintaining oxidation resistance, but the development process is a lengthy one. This is mostly due to the difficulties of predicting the creep strength of newly developed alloys. Physical real-time creep tests are expensive and offer limited practical use during a time-restricted development phase.

Consequently, the ability to better predict the service life of new materials and alloys is generally desired. Creep models attempt to achieve this goal by either relying on simple extrapolations or performing complex physically based calculations.

1.1. State of the art

Reliable prediction of the true creep resistance is a challenging task. A wide range of different creep models were developed and refined over time. They can be essentially sorted in the following two categories:

(a) Extrapolations and phenomenological approaches:

These models usually take existing creep data as a starting point and do not consider interactions within the material.

A set of fit-parameters describes the creep behaviour at one specific set of conditions of one defined material. Once they manage to accurately conform to the experimental data, the extrapolation of the calculations to the ultimate lifetime (until failure of the material) is achievable.

This strategy seems very practical, but extrapolations are only accurate over a narrow range of parameter values. The reliability will strongly rely upon the magnitude of change introduced by influencing factors like stress and temperature as well as the

prevalent microstructure. Usually the predicted results have to include sufficiently wide safety margins.

A strategy to circumvent these tight restrictions is to consider mechanistic phenomena within the structure of the material which leads to:

(b) Physical and mechanistic models:

As soon as a model is based on measurable physical values in addition to creep rate or lifetime, the model's accuracy with respect to the parameter changes regarding the material and the surrounding system can be significantly enhanced.

Ideally, the material's thermal and mechanical history during production can be incorporated into the simulation. Such a model provides a link between its (start-)microstructure and its macroscopic properties. The microstructural evolution would also serve as a second reference for later model evaluation.

1.2. Aim of this work

This thesis focuses on further improvement of the existing semi-physical SRKS creep model (Sonderegger-Riedlsperger-Krenmayr-Schmid) from May 2018 and its implementation in the Matlab environment. [1]

To begin with, a brief overview of already existing models on creep and the necessary ingredients for such models is given.

The material used in the model is a specific P91 weld material provided by the project partner. The weld material is not to be confused with the fine grain heat affected zone in near proximity to the weld zone.

Further tasks are to create several new MatCalc scripts for MatCalc 6.01 to calculate the chemical composition of the matrix as well as the composition and temporal evolution of the precipitates during service. The latter one will be partially based on existing MatCalc 5.62 scripts.

Additionally, the currently used equations and the Matlab-code (which serves as the framework) will be reviewed and enhanced. For instance, this includes modifications of the user interface, code streamlining, better handling of multiple datasets and fit-parameter sets, the graphical output of the time to rupture diagram and other minor changes.

Finally the changes and results will be summarised, reviewed and discussed.

2. Literature and preliminary models

This chapter is meant to give an overview of the principles of creep mechanisms, P91 steel, and preliminary work done in the field of creep modelling. This includes diverse sources from literature as well as the very extensive work done on creep modelling by the IMAT-modelling team on whose results this thesis is based.

2.1. Mechanisms and appearance of creep

Creep can be defined as a time- and temperature-dependent plastic deformation of materials under load. [2]

Various materials show distinctive varying behaviours when exposed to different temperatures. At low temperatures, the deformation under stress corresponds approximately to a function of the applied stress $\epsilon = f(\sigma)$. At elevated temperatures (30% to 40% of the melting point T_m in Kelvin), the resulting deformation corresponds to a function which itself depends on the stress, time and temperature $\epsilon = f(\sigma, t, T)$. This diverging behaviour can be attributed to thermally activated processes. [3, 4]

The dominant deformation processes at a given combination of temperature and shear stress can be seen in so called 'deformation mechanism diagrams'. One of the most well known of its kind is the Ashby deformation map as seen in (Figure 2.1). [5]

Even though the creep deformation mechanisms are in principle the same for different materials, the specific deformation maps differ greatly for e.g. aluminium based alloys or ceramics. [2]

For example, at high temperatures and low stresses, diffusional flow is the main deformation mechanism, albeit at a very low total deformation rate. Usually grain boundaries serve as sources and drains of atoms and vacancies during the creep process. The vacancies diffuse to places where higher compressive stress or lower tensile stress are present. As a result, the material flow occurs in the opposite direction. [2, 6, 7]

If the applied stress is increased, the importance of dislocations for total creep increases and becomes more pronounced. This is mostly the case in crystalline materials with also relatively high specific homologous temperatures [8]. As soon as a moving dislocation reaches an obstacle, e.g. a precipitate, it is mechanically hindered in further movement. At elevated temperatures, the dislocation can evade an obstacle by means of thermally activated dislocation climbing. [2]

At even higher stresses, the classic plastic deformation occurs up to the theoretical strength of the material. This dislocation slip that characterizes conventional plastic

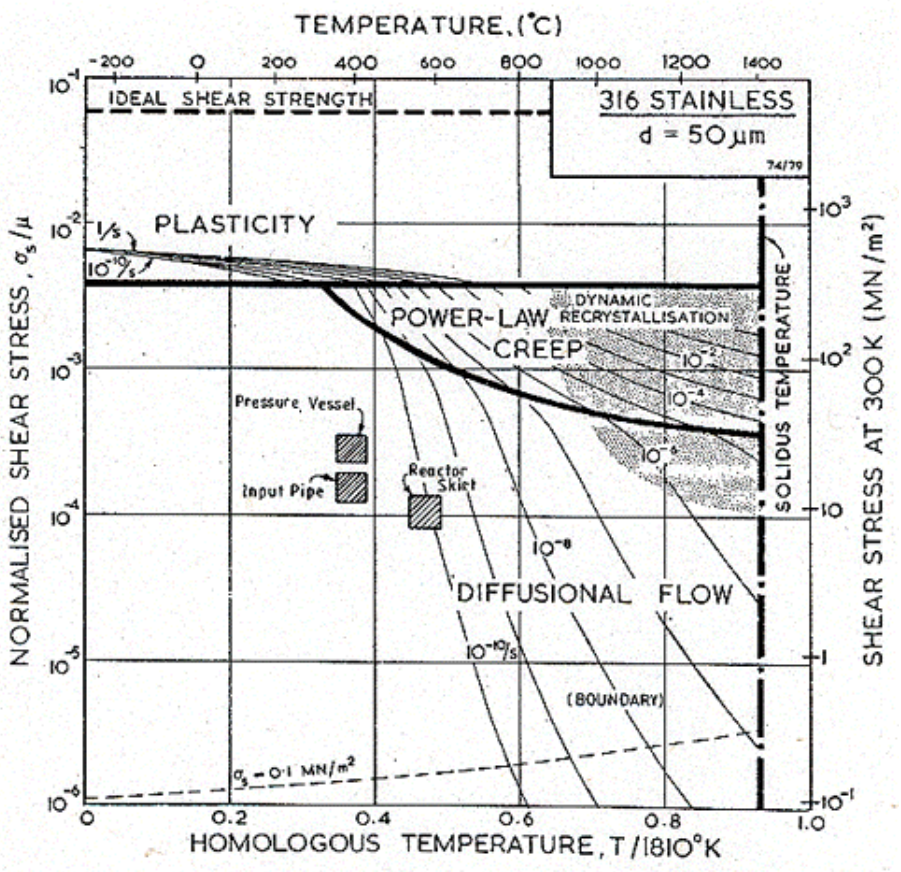

Figure 2.1.: Ashby deformation map [5]

deformation prevails in the entire temperature range, provided that the stress is high enough to exceed the yield strength. [3, 6]

In addition to the mechanisms above, high temperatures allow the grains in metals and ceramics to directly move by each other. This grain boundary sliding is not shown in the deformation mechanism map because its total contribution to creep deformation is negligible in metals. [3, 6]

Despite the rather small contribution to creep deformation, it is still very important that grain boundaries stay resistant to grain boundary sliding. The displacement of whole grain boundaries can lead to a strong increase in local stress, especially at points where three grain boundaries meet. This local increase can lead to a rupture of the local grain boundaries and dissection of the grains. Countering this, during grain boundary sliding, diffusional creep ensures the connectivity between grains. If the diffusional flow is high enough, the danger of premature material damage by cracking is lowered. [2, 3, 6]

Figure 2.2 shows an exemplary creep curve. At given stress σ, ϵ_t shows the total strain over time. ϵ_t consists of the instantaneous strain ϵ_i and the creep strain ϵ_c. t_T is the point of initiation of the tertiary creep regime, t_R is the final time to rupture. [9]

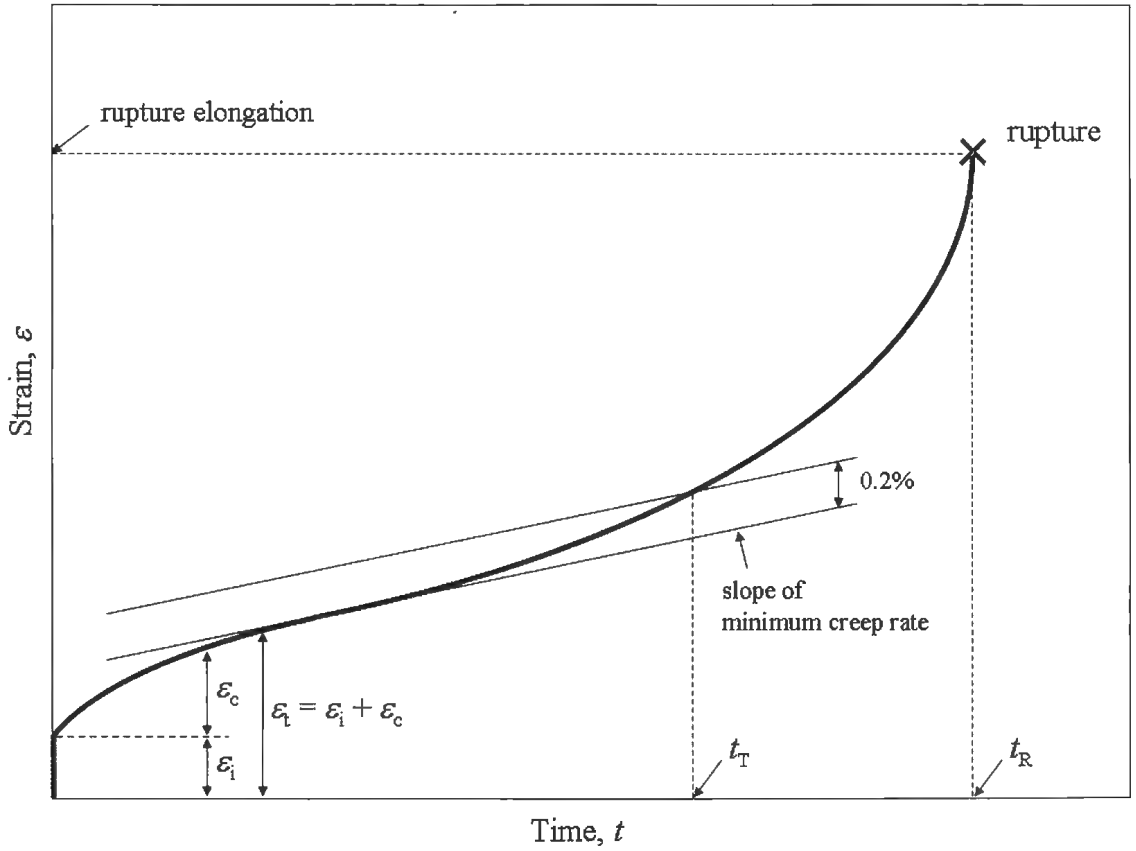

Figure 2.2.: Creep curve from NIMS [9]

Generally speaking, a creep curve can be divided into three distinctive regimes: Primary, secondary and the already mentioned tertiary creep.

During primary creep (as shown in Figure 2.2 up to about the point near ϵ_c) mainly material strengthening effects occur and the creep rate decreases steadily. [3, 4, 6]

After that, during the secondary creep stage, there is an equilibrium between thermally activated processes and the material strengthening mechanisms. This results in a fairly constant creep rate up to point t_T which is defined as the point where the tertiary creep regime starts. [9]

As can be seen in figure 2.2, the starting point t_T is located at the point of time where the strain of the actual creep curve deviates more than 0.2% from the slope of minimum creep rate. [9]

The tertiary creep regime is dominated by a strong increase in creep rate. This is mainly due to softening processes in the material, such like the fast development of creep voids. This results in a strongly accelerated creep until fracture. [3, 4]

The resulting rupture times from many different creep curves with varying stresses and temperatures can be plotted in one unified 'time to rupture'-diagram to give a very good overview. Figure 2.3 shows such a TTR Diagram for experimentally gathered data for martensitic steel P92: [10]

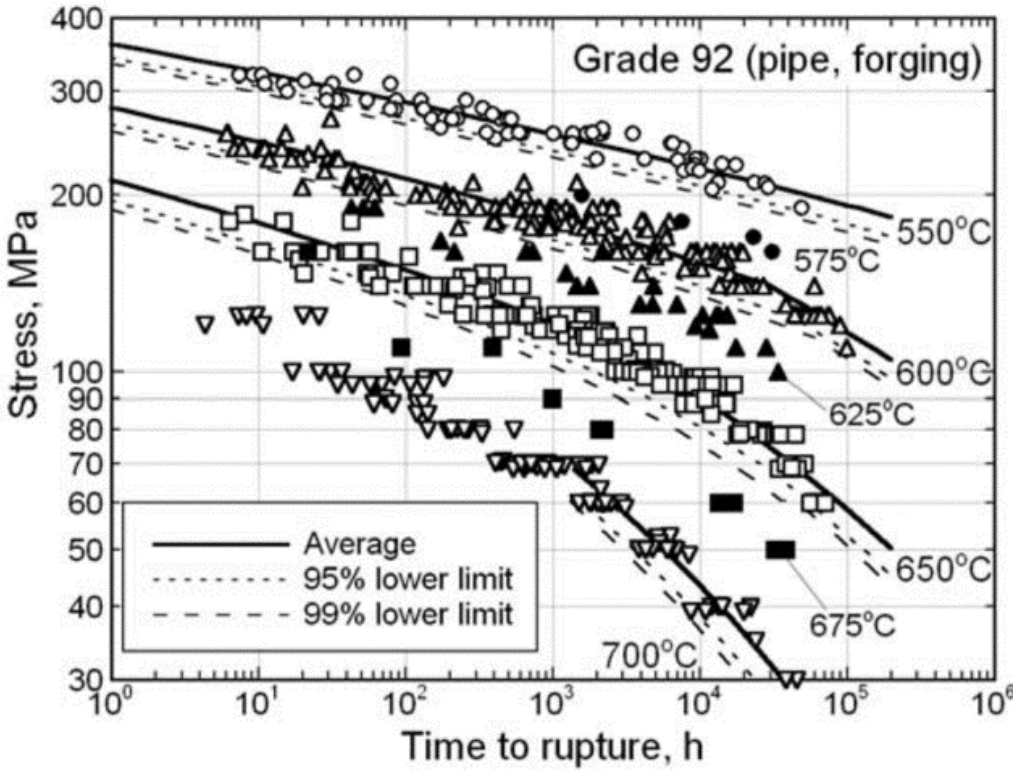

Figure 2.3.: ASME TTR-diagram [10]

Such a diagram is the result of many very time consuming experiments, each data point represents one creep experiment. Especially noting the logarithmic scaling of the diagram, the scattering of the final time to rupture for one and the same material is apparent.

Also the effect of relatively slight variations in temperature is shown by vastly differences in service life of the material until failure. For example, at 200 MPa the material ruptures after only minutes at 650°C, after over one month at 600°C and lasts for many years at 550°C.

2.2. Martensitic steel P91

'Grade 91 alloy steel' is an acronym for the ferritic-martensitic steel X10CrMoVNb9-1.

The main alloying components are 9% chromium, 1% molybdenum as well as vanadium and niobium as micro-alloying components. The steel has a controlled nitrogen content according to ASTM A 335, A 213 or to EN 10216-2 [11].

The letters in P91 or T91 refer to the shape in which the steel is produced, namely pipes or tubes.

This specific martensitic steel is often the material of choice in fossil-fuelled power plants. It is mainly used for high-temperature applications like reheater and superheater tubes, headers and steam piping.

The main advantages are a relatively high toughness, good stability against oxidation, high creep strength, low thermal expansion and high thermal conductivity. All these properties combined allow higher resistance to thermal fatigue compared to other steels. This is achieved while maintaining relatively low material and production costs in comparison to austenitic steels and nickel-base alloys. [12, 13, 14, 15, 16, 17, 18, 19, 20]

The table in figure 2.4 shows the specific chemical composition of three typical Grade 91 steels [9]. The experimentally determined creep curves of these materials will later be used as references for the model evaluation. MgA and MgB share the same chemical composition, but undergo different heat treatments as shown in figure 2.5.

NIMS reference code	Chemical composition (mass percent)[1)]											
	C	Si	Mn	P	S	Ni	Cr	Mo	V	Al*	N	Nb*
Requirement[2)]	0.08 - 0.12	0.20 - 0.50	0.30 - 0.60	≤0.020	≤0.010	≤0.40	8.00 - 9.50	0.85 - 1.05	0.18 - 0.25	≤0.04	0.030 - 0.070	0.06 - 0.10
MgA	0.08	0.34	0.49	0.005	0.004	0.09	8.34	0.89	0.23	0.011	0.059	0.070
MgB												
MgC	0.10	0.24	0.44	0.005	0.001	0.04	8.74	0.94	0.21	0.014	0.0582	0.076

1) The chemical composition given above was reported by the steel manufacturers except for the elements marked with asterisk, for which the analysis was carried out at NIMS.
2) ASME SA-387/SA-387M Grade 91-2004, "SPECIFICATION FOR PRESSURE VESSEL PLATES, ALLOY STEEL, CHROMIUM-MOLYBDENUM"

Figure 2.4.: Chemical composition (product analysis) of P91 steel plates [9]

The table in figure 2.5 lists the production specifics and thermal history for the NIMS-reference grade 91 steels [9]. The MgA, MgB and MgC shown in the TTR-diagrams (e.g. figure 5.23 on page 46) correspond with these two tables in figures 2.4 and 2.5.

The main objective of the heat treatment is to get an optimally balanced ratio between toughness and high-temperature strength. The whole heat treatment (austenitisation, cooling and stress relieving) has to be carried out within tight tolerance limits in order to achieve a high degree of stability later on which depends on the creation of a satisfying martensitic microstructure. [21]

NIMS reference code	Type of melting [2]	Size of ingot (kg)	Deoxidation process	Product form	Dimensions [3] (mm)	Processing and thermal history	Austenite grain size number [4]	Rockwell hardness (HRC)	Non-metallic inclusion [5] (%)
MgA [6]	BEA	13 500	Al-Si-killed	Plate	25 T 2 150 W 9 477 L	Hot rolled 1 050℃/10min AC 770℃/60min AC 740℃/8.4h FC [7]	9.0	13	dA = 0.00 dB = 0.00 dC = 0.02
MgB [8]						Hot rolled 1 050℃/10min AC 770℃/60min AC 740℃/60min FC [7]		14	
MgC	LDC	20 000			50 T 2 200 W 15 000 L	Hot rolled 1 060℃/90min AC 760℃/60min AC 730℃/8.4h FC	8.7	17	dA = 0.00 dB = 0.02 dC = 0.01

1) The plates were sampled in 1988 and 1991. Details other than grain size number, hardness and non-metallic inclusion are as reported by the steel manufacturers.
2) BEA : basic electric arc furnace, LDC : LD converter
3) T : thickness, W : width, L : length
4) JIS G 0551-2005, "Steels - Micrographic determination of the apparent grain size"
5) JIS G 0555-2003, "Microscopic testing method for the non-metallic inclusions in steel"
6) This material is the same heat as that in NRIM Fatigue Data Sheets No.78(1993).
7) The stress relieving heat treatment was performed at NRIM.
8) This material is the same heat as the MgA except for the thermal history.

Figure 2.5.: Details of NIMS P91 steel plates [9]

If the cooling rate is too slow, α - Ferrite is formed, but usually for components with a diameter under 500 mm cooling by air is sufficient. [21, 22, 23]

The formation of either lath- or plate-martensite during cooling after austenitisation depends on the carbon content. [21, 23, 24, 25, 26, 27]

The further microstructural evolution of P91 including the precipitates during production and service will be discussed in more detail in the next chapter.

2.3. Microstructure of P91

Unlike ideal crystals, real crystals show many defects and variations within their inner structure. These deviations from a perfect arrangement of atoms lead to a distortion of the crystal lattice. This subsequently increases the inner energy of the crystal. These crystal 'defects' are not necessarily a negative thing, the creation of specific defects determines and even improves certain material properties. [4]

Crystal defects can be summarised into these categories classified by their geometric dimensions: [28]

- Zero-dimensional point defects: vacancies, interstitial and substitutional atoms
- One-dimensional line defects: (screw- and step-)dislocations
- Two-dimensional surface defects: grain boundaries (high and low angle), twin boundaries, phase boundaries, surface boundaries and also stacking faults.
- Three-dimensional spatial defects: precipitates, inclusions, pores and cavities

The high creep resistance of 9-12% Cr steels results from its precipitate-stabilized microstructure (a variation of all previously mentioned defects) and is illustrated in figure 2.6. [29]

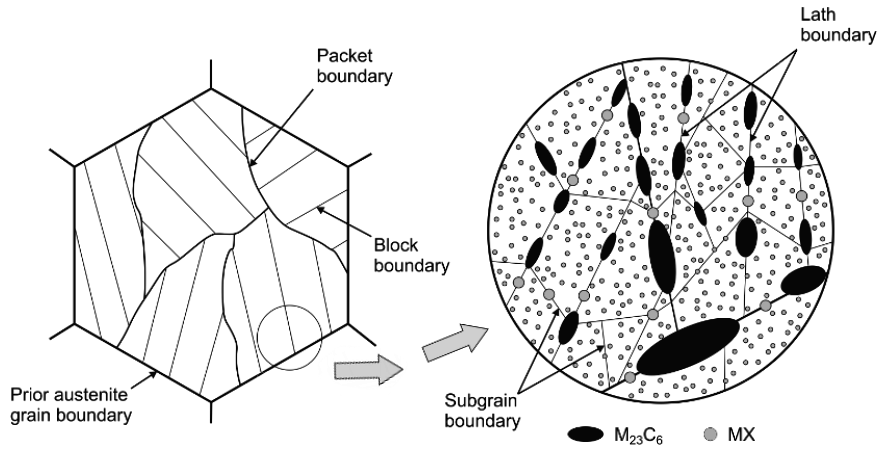

Figure 2.6.: Microstructure, modified from [29]

The main features are the prior austenite grain boundaries (PAGB), the martensite laths and their boundaries as well as all low angle grain boundaries (subgrain boundaries).

The most important precipitates are:

(a) Chromium carbides: $M_{23}C_6$

They precipitate during tempering on the prior austenitic grain boundaries as well as on other grain boundaries. [21, 25]

At elevated temperatures, the high coarsening tendency (which leads to a decrease in number density) has a negative effect on the creep strength. [12, 14, 29, 30]

(b) MX phases $(Nb, V)(C, N)$

This class of precipitates includes NbC, VN and other mixed form variations. These precipitates form mostly at subgrain boundaries and dislocations. Their tendency to coarsening is comparatively low and also contributes to the reinforced creep resistance. [12, 14, 29, 30]

(c) Aluminium nitrides AlN

Aluminum nitrides have a negative influence regarding to long-term creep resistance but they are present in small amounts because of their positive influence on the manufacturing process. [12, 31, 32]

(d) Laves phase $(Fe, Cr, Si)_2(W, Mo)$

The laves phase usually occurs after several hundred hours of service and its role in influencing the creep strength is controversially discussed. They usually precipitate at grain boundaries or subgrain boundaries and also show a high rate of coarsening. [12, 14, 30, 33]

(e) Modified Z-phase $Cr(V, Nb)N$

The formation of modified Z-phase at expense of MX after long-term creep results in a creep strength decline.

The improved creep strength by the general presence of the precipitates is mainly due to following effects: [21, 34, 35]

- hindering of dislocation movements
- pinning or restricting the movements of subgrain boundaries

Information about size and chemical composition of precipitates in real samples can be acquired by means of SEM and TEM-investigations.

Most information about grain- and subgrain-sizes can be derived by means of EBSD-measurements as described in the next chapter.

2.4. Creep models

The advantage of creep modelling lies in the possibility of predicting the deformation of a component at a certain point in its time of life. In general, literature distinguishes between 'phenomenological' and 'semi-physical' creep models. In some cases, a creep model shows characteristics of both variants.

2.4.1. Phenomenological creep models

Phenomenological models usually are built on analytic functions to describe the occurring creep deformation and to predict the lifetime of a material.

These functions are supported by results of macroscopic creep tests but do not consider specific creep mechanisms. Consequently, they rely heavily on experimentally ascertained fit-parameters. These parameters will vary by changing stress, temperature, type and thermal history of the material, which often limits the usefulness of these models.

As long as these parameters stay close to the initial experimental conditions, they can be of practical use with good accuracy.

The most widely used approaches for predicting the service time for materials are the so-called extrapolation methods. Well-known extrapolation methods have first been developed by Monkman and Grant [36] in 1956 and Larson and Miller [37] in 1952. [38, 39]

Once the appropriate fit-parameters are fixed, they are very easy to apply. However, their utilisation is limited to cases similar to the conditions for which the assessment has been carried out.

Since the scatter in the result of creep experiments is usually high, a significant number of creep tests has to be performed. Otherwise, the accuracy of the results will strongly deteriorate [40].

Usually the experiments are carried out for short-term creep loads, often in the range of 10^3 hours (41 days) or a little bit longer. This data is then extrapolated to long-term conditions as long as 10^5 hours (11.4 years). This extrapolation ignores the microstructural evolution or even change of creep mechanisms during the materials service. The extrapolation will lose accuracy and predictability due to these systematic errors.

While Monkman-Grant and Larson-Miller only predict the material's ultimate lifetime, other phenomenological models show either the strain or the strain rate at a specific point of time.

Many of these models concentrate on a specific creep regime: [38, 39]

- Valid only for the primary creep regimes are the models of McVetty [41], Conway [42], Phillips [43] and Graham-Walles [44].
- Nadai [45] and Norton [46] place their focus on the secondary regime.

- The models of McHenry [47], Rabotnov [48] and Sandström-Kondyr [49] are all functional up to the tertiary creep regime.

According to Holdsworth et al. [50], the Modified Graham-Walles Model [44, 50], the Bolton Characteristic Strain Model [51] as well as the MHG Model [52, 53, 54] yield the best results for P91 steel. [38, 39]

Justifiably, the question arises to what extent these models are predictions or just a fit of data sets. For example, the Extended Omega Model, which shows an excellent agreement between experimental strain rates and calculated creep curves, has a total of twelve fit parameters. [55, 56]

These fit parameters are freely adjusted using a series of creep curves from experiments at different temperatures and stresses. None of the fit parameters can be measured independently of the creep experiment, and the physical interpretation is sometimes unclear. Because of this, it is very difficult to define the limits of the models but they can be used as numerically inexpensive tool for implementation in finite element simulations of components. [39]

Even after successful application, the model does not provide any information about the underlying reasons for good or bad creep behaviour. This microstructural or micromechanical information would be needed for the optimization of materials or their production process or even development of new alloys.

2.4.2. Physical based creep models

In contrast to phenomenological creep models, semi-physical models potentially include the microstructure of the material and its evolution during service. This provides a link between macroscopic properties and the microstructure even during episodes with varying stresses and temperatures.

Due to these properties, the predictability of a semi-physical creep model extends much further. What has to be considered are considerably longer calculation times and the impact of an incomplete integration of the microstructure due to the high complexity.

Nevertheless, semi-physical models are the only option at the time for understanding the impact of the starting microstructure on creep properties.

The differences in starting microstructure may originate from different chemical compositions as well as the complete thermal history during production. This includes welding and all other heat treatments like austenitization and quenching.

If reasonably complete in terms of creep phenomena and set up correctly, a physical based creep model can consider these effects.

The current work is based on a hybrid model by Yadav et al. [57] where Yadav combines the detailed (semi-)physical dislocation model by Ghoniem [58] for primary and secondary creep with an added model for continuum damage mechanics (CDM) in the tertiary creep regime by Basirat [59].

Ghoniem's model contains rate equations for dislocation densities, subgrain sizes and elongation. The evolution of each microstructural constituent is coupled with the status of each other constituent.

Basirat introduced his CDM-model especially for the application on martensitic 9-12% Cr steels in 2012. As an addition, not only dislocations are considered, but also the coarsening of $M_{23}C_6$ precipitates as well as solid solution depletions due to the formation of Laves phase and the formation of creep voids [30]. In addition to the damage progression, Basirat also considers the evolution of dislocations according to preceding efforts of Blum [60].

The following simplifications and extensions have been considered by Yadav et al. for this combination:

- Since the equilibrium phase fraction of Laves phase is usually reached within a few days and then remains constant throughout the entire creep process after, the formation of this phase is no longer considered as a damage mechanic.
- Carbide coarsening and the formation of creep voids remain as the only damage parameters, which are included as proposed by Basirat.

To improve computational time, mechanisms which have proven to have a very low effect were neglected:

- The emission of dislocations from the subgrain walls on the evolution of dislocation densities
- Nucleation of new subgrains was found to have a negligible effect on the subgrain size evolution

Whereas in the model of Ghoniem all precipitates have equal diameter, Yadav extended the model to potentially include precipitates of different size classes.

2.4.3. IMAT creep model

The current approach in this work is based on a further developed version of the hybrid model of Yadav by Sonderegger-Riedlsperger-Krenmayr-Schmid in 2018. [1, 38, 39, 61]

This SRKS model 2018 is based on work of Yadav from 2016 [57] and proves to be a substantial leap in regard of involving MatCalc precipitate evolution during service time as well as eliminating substantial errors in the model.

Schmid included the option to include data of the microstructural evolution of precipitates by coupling the model with results from precipitation kinetic software, in this case 'MatCalc'. [1]

All governing equations used in that model and the enhancements carried out in the course of this thesis are listed in the next chapter 3.

3. Creep model governing equations

In this chapter all equations used in the model and the experimental part of this thesis are listed and explained. At the end of each paragraph the corresponding line numbers to the MATLAB-code are referenced wherever applicable.

Figure 3.1 represents a schematic flow chart diagram for the connection of all equations in this creep model. At first, the microstructural starting condition has to be initialized (red octagonal box).

Then, for each iteration step, all variables are updated in the indicated order until the creep deformation rate $\dot{\varepsilon}$ is calculated for the selected time interval. All other variables that describe the changed system state (e.g. dislocation densities or subgrain size) are saved and used as starting values for the next iteration step.

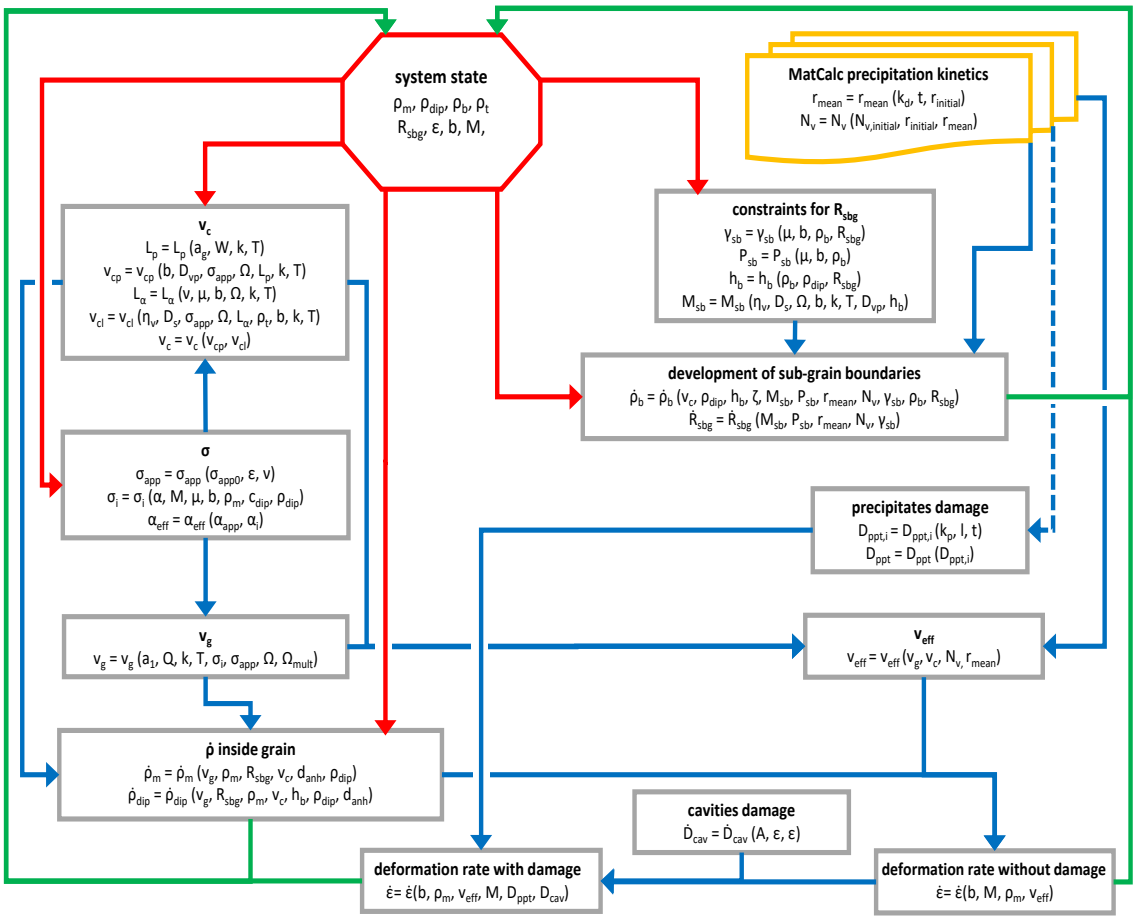

Figure 3.1.: Schematic sequence of creep simulation

The basis for all calculations is the original Orowan equation, eq. 3.1 which describes the creep strain rate via the density development of mobile dislocations and the effective dislocation velocity. (MATLAB ref.: page 123, line 302)

$$\frac{d\varepsilon}{dt} = \frac{b \cdot \rho_m \cdot v_{eff}}{M} \tag{3.1}$$

The modified Orowan equation (Eq. 3.2) describes the strain rate by basically extending Orowan's equation (Eq. 3.1) with damage parameters derived from precipitates (D_{ppt}) and cavities (D_{cav}). (MATLAB ref.: page 123, line 288)

$$\frac{d\varepsilon}{dt} = \frac{b \cdot \rho_m \cdot v_{eff}}{M\left(1 - D_{ppt}\right)\left(1 - D_{cav}\right)} \tag{3.2}$$

All microstructural elements show a temporal evolution which have to be subdivided into terms of source, transformation or annihilation.

During the creep experiment, the diameter of the sample is reduced. At defined initial load, the stress per area would increase over time. To keep the stress constant, it has to be corrected (Eq. 3.3). Beside the calculated lateral strain, one has to define the Poisson number, where ν=0.3 is fitting for most metals. (MATLAB ref.: page 120, line 66)

$$\sigma_{app} = \sigma_{app_0}\left(1 + \nu \cdot \varepsilon\right) \tag{3.3}$$

Equation 3.4 for the dislocation glide velocity by Čadek 1988 [62] is the basis for the further developed equation 3.6.

$$v_g = a \cdot \sigma_{eff} \cdot \frac{\Omega}{k_B \cdot T} \cdot \exp\left(\frac{-Q}{k_B \cdot T}\right) \tag{3.4}$$

In the improved version of the model, equation 3.5 describes the inner stress (backstress) used for the deprecated σ_{eff} but is also used in equation 3.6 to calculate v_g. (MATLAB ref.: page 120, line 69)

$$\sigma_i = \alpha \cdot M \cdot G \cdot b \cdot \sqrt{\rho_m + c_{dip} \cdot \rho_{dip}} \tag{3.5}$$

One innovation in the model is the modification of the former back stress concept for calculating the sliding velocity of dislocations. In cases of low applied stresses the models of Ghoniem [58] and Yadav [57] yield negative effective stresses (by $\sigma_{eff} = \sigma_{app} - \sigma_i$) and thus negative sliding velocities occurred even with positive applied external stress.

The dislocation glide velocity (Eq. 3.6) is formulated by the probability of a forward and a backward motion by an Arrhenius approach. a_1 and Ω_{mult} are fitted, both variables and their values will be discussed in chapter 6. (MATLAB ref.: page 120, line 80)

$$v_g = a_1 \cdot \exp\left(-\frac{Q}{k_B \cdot T}\right) \cdot \exp\left(-\frac{\sigma_i \cdot \Omega \cdot \Omega_{mult}}{k_B \cdot T}\right) \cdot 2 \cdot \sinh\left(\frac{\sigma_{app} \cdot \Omega \cdot \Omega_{mult}}{k_B \cdot T}\right) \tag{3.6}$$

In order to link the interactions of mobile dislocations with precipitates within subgrains, the glide velocity of dislocations was substituted by the new equation for 'effective velocity' (Eq. 3.7). This effective speed includes a combination of climbing and gliding speed, with climbing speed being proportional to the amount of precipitates to climb. (MATLAB ref.: page 122, line 213)

$$\frac{1}{v_{eff}} = \frac{1}{v_g} + \frac{\pi}{2 \cdot v_c} \cdot \sum_{i=1}^{n} N_{v,i} \cdot r_{mean,i}^3 \tag{3.7}$$

The equation for mobile dislocations (Eq. 3.8) contains Frank-Read sources and the generation from subgrain boundaries as generation terms. Both recovery by climbing and dynamic recovery are possible, furthermore reduction by the formation of subgrain boundaries takes place. (MATLAB ref.: page 123, line 269)

$$\frac{d\rho_m}{dt} = \underbrace{v_{eff} \cdot \rho_m^{3/2}}_{\text{Frank-Read-source}} + \underbrace{\frac{v_{eff} \cdot \beta \cdot R_{sg}}{h_b^2}}_{\text{emission on subgrain boundaries}} - \underbrace{\frac{v_{eff}}{2 \cdot R_{sg} \cdot \rho_m}}_{\text{generation of subgrain boundaries}} - \underbrace{8 \cdot \rho_m^{3/2} \cdot v_{cc}}_{\text{recovery by climbing}} - \underbrace{\rho_m \cdot v_{eff} \cdot d_{anh} \cdot \left(\rho_m + \rho_{dip}\right)}_{\text{dynamic recovery}} \tag{3.8}$$

The development of dipole dislocations (Eq. 3.9) is composed of the immobilization of mobile dislocations at subgrain boundaries and recovery through climbing and dynamic recovery. (MATLAB ref.: page 123, line 274)

$$\frac{d\rho_{dip}}{dt} = \underbrace{\frac{v_{eff}}{2 \cdot R_{sg} \cdot \rho_m}}_{\text{immobilization on subgrain boundaries}} - \underbrace{\frac{8 \cdot v_{cc}}{h_b \cdot \rho_{dip}}}_{\text{recovery through climbing}} - \underbrace{\rho_m \cdot v_{eff} \cdot d_{anh} \cdot \rho_{dip}}_{\text{dynamic recovery}} \tag{3.9}$$

The evolution of boundary dislocations (Eq. 3.10) can be divided into two terms. One for the transformation of dipole dislocations into boundary dislocations and the other for formation of new subgrain interfaces. (MATLAB ref.: page 122, line 204)

$$\frac{d\rho_b}{dt} = \underbrace{\frac{(8-\zeta) \cdot \rho_{dip} \cdot v_{cc}}{h_b}}_{\text{static recovery and loss of dipoles}} - \underbrace{\frac{M_{sgb} \cdot \rho_b}{R_{sg}} \cdot \left(P_{sgb} - 2 \cdot \pi \cdot \gamma_{sgb} \cdot \sum_{i=1}^{n} r_{mean,i}^2 \cdot N_{v,i}\right)}_{\text{annihilation through subgrain growth}} \tag{3.10}$$

The subgrain growth (Eq. 3.11) is driven by the diffusion-induced subgrain mobility and a growth pressure to minimize the elastic energy of the system. By contrast, precipitations slow down and dampen potential subgrain growth via the Zener pinning effect. [57] (MATLAB ref.: page 122, line 209)

$$\frac{dR_{sg}}{dt} = M_{sgb} \cdot \left(\underbrace{P_{sgb}}_{\substack{\text{growth} \\ \text{pressure}}} \underbrace{- 2 \cdot \pi \cdot \gamma_{sgb} \cdot \sum_{i=1}^{n} r_{mean,i}^2 \cdot N_{v,i}}_{\text{Zener backpressure}} \right) \tag{3.11}$$

The approach for an equation of cavitation softening (Eq. 3.12) has been adapted from Basirat et al. [63] and Yin-Faulkner [64]. For a more detailed description of these, see Yadav et al. [57, 65]. (MATLAB ref.: page 124, line 326)

$$\dot{D}_{cav} = A \cdot \varepsilon \cdot \dot{\varepsilon} \tag{3.12}$$

The path length for diffusion along the dislocation core is described by equation 3.13, including the size of the elementary cell a_g. (MATLAB ref.: page 120, line 86)

$$L_p = a_g \cdot \sqrt{2} \cdot \exp\left(\frac{W}{2 \cdot k_B \cdot T} \right) \tag{3.13}$$

Equation 3.14 calculates the climb velocity for pipe diffusion. (MATLAB ref.: page 120, line 89)

$$v_{cp} = \frac{2 \cdot \pi \cdot b \cdot D_{vp} \cdot \sigma_{eff} \cdot \Omega}{L_p^2 \cdot k_B \cdot T} \tag{3.14}$$

The distance between interacting dislocation and lattice error L_α is calculated as shown in equation 3.15. This variable is needed to calculate the climbing speed by lattice diffusion. (MATLAB ref.: page 120, line 93)

$$L_\alpha = \frac{(1+\nu) \cdot G \cdot b \cdot 0.5 \cdot \Omega}{(1-\nu) \cdot 3 \cdot \pi \cdot k_B \cdot T} \tag{3.15}$$

Equation 3.16 now describes the climbing speed by lattice diffusion. (MATLAB ref.: page 120, line 96)

$$v_{cl} = \frac{2 \cdot \pi \cdot \eta_v \cdot D_s \cdot \sigma_{eff} \cdot \Omega}{\left[1 - \eta_v \cdot \ln\left(L_\alpha \cdot \sqrt{\rho_t}\right)\right] \cdot b \cdot k_B \cdot T} \tag{3.16}$$

The climb velocities as a sum of climbing by lattice diffusion and pipe diffusion are described in equation 3.17. (MATLAB ref.: page 120, line 100)

$$v_c = v_{cp} + v_{cl} \tag{3.17}$$

Equation 3.18 describes the interfacial energy of subgrain boundaries. (MATLAB ref.: page 120, line 103)

$$\gamma_{sgb} = \frac{1}{3} \cdot G \cdot b^2 \cdot \rho_b \cdot R_{sg} \tag{3.18}$$

The subgrain growth pressure is defined by equation 3.19. (MATLAB ref.: page 120, line 106)

$$P_{sgb} = \frac{4}{3} \cdot G \cdot b^2 \cdot \rho_b \tag{3.19}$$

Equation 3.20 describes the dislocation spacing within the subgrain boundary (MATLAB ref.: page 120, line 109)

$$h_b = \frac{1}{\left(\rho_b + \rho_{dip}\right) \cdot R_{sg}} \tag{3.20}$$

If the inequation 3.21 is fulfilled, the mobility of the subgrain boundaries M_{sgb} is calculated by Eq. 3.22, otherwise by Eq. 3.23. (MATLAB ref.: page 122, line 191)

$$P_{sgb} \geqslant 2 \cdot \pi \cdot \gamma_{sgb} \cdot \sum_{i=1}^{n} r_{mean,i}^2 \cdot N_{v,i} \tag{3.21}$$

Equation 3.22 for mobility of subgrain boundaries (MATLAB ref.: page 122, line 193)

$$M_{sgb} = \frac{2 \cdot \pi \cdot \eta_v \cdot D_s \cdot \Omega}{b \cdot k_B \cdot T} + \frac{2 \cdot \pi \cdot b \cdot D_{vp} \cdot \Omega}{h_b^2 \cdot k_B \cdot T} \tag{3.22}$$

Equation 3.23 for mobility of subgrain boundaries (MATLAB ref.: page 122, line 200)

$$M_{sgb} = \frac{D_s \cdot \Omega}{2 \cdot \pi \cdot k_B \cdot T \cdot \sum_{i=1}^{n} r^4_{mean,i} \cdot N_{v,i}} \tag{3.23}$$

Calculation of the damage parameter by precipitate coarsening by Eq. 3.24, where l=6 for MX-type precipitates and l=4 for metal carbides. (MATLAB ref.: page 124, lines 321-322)

$$D_{ppt,i} = 1 - \sqrt[1-l]{k_p \cdot t + 1} \tag{3.24}$$

Damage rate expressed as rate equation 3.25 as an alternative form of Eq. 3.24.

$$\dot{D}_{ppt,i} = \frac{k_p}{l-1} \cdot \left(1 - D_{ppt,i}\right)^l \tag{3.25}$$

The complete damage by coarsening (Eq. 3.26) is the sum of all damages through precipitaton specific coarsening rates. (MATLAB ref.: page 124, line 323)

$$D_{ppt} = \sum_{i=1}^{n} D_{ppt,i} \tag{3.26}$$

The coarsening of precipitates at constant volume fraction is referred to as 'Ostwald-ripening' and is calculated by equation 3.27. $r_{initial}$ refers to the original precipitation radius, r_{mean} to the precipitation radius at time t, while k_d is a temperature-dependent variable for the coarsening rate. [6]

$$r^3{}_{mean} + r^3{}_{initial} = k_d \cdot t \tag{3.27}$$

Due to the coarsening of the precipitates under the assumption of a constant volume, the number of precipitates per volume N_V changes. Equation 3.28 describes this relation, where $N_{V,initial}$ is the initial number of precipitates per volume.

$$N_V = \frac{N_{v,initial} \cdot r^3{}_{initial}}{r^3{}_{mean}} \tag{3.28}$$

The diffusion coefficients D_s and D_{vp}, which are primarily required for the equations 3.16, 3.22 and 3.23, are calculated as shown in equation 3.29.

$$D = D_0 \cdot \exp\left(-\frac{Q}{R \cdot T}\right) \tag{3.29}$$

The calculated diffusion coefficients applied in this thesis are reused and taken from the work of Schmid 2018, the detailed deviation can be read there at chapter 2.5 [1].

All constants and the values of other variables and fit-parameters used are listed in table 4.4 on page 24.

4. Methods and experimental work

This chapter gives an overview over all experimental efforts done over the course of the thesis and specifies all parameters to replicate the work.

4.1. Experimental material and input data

Table 4.1 lists all sample specimens available for analysis. It has to be noted, that only data of BOA 1 by means of EBSD analysis was made use of for gaining information about the starting microstructure needed for the creep model.

Table 4.1.: Specimen reference table for P91 weld material creep samples

name	attributes
BOA 1	unaltered weld material
BOA 2.1	creep-loaded at 575°C
BOA 2.2	thermally aged at 575°C
BOA 3.1	creep-loaded at 600°C
BOA 3.2	thermally aged at 600°C
BOA 4.1	creep-loaded at 625°C
BOA 4.2	thermally aged at 625°C

Experimentally ascertained creep curves and rupture time data was collected from different sources. These curves are plotted as experimental references in the creep- and TTR-diagrams later (e.g. 5.20 on page 44). Table 4.2 lists and references the original sources.

Table 4.2.: Reference table for source of experimental TTR-curves

short	full name	reference
ASME	American Society of Mechanical Engineers	[66]
ECCC	European Creep Collaborative Committee	[67]
NIMS	National Institute for Materials Science	[9]
P91 weld	voestalpine Böhler Welding	email correspondence

The values in table 4.3 were used as the microstructural starting parameters in all Matlab creep model calculations. All them were directly adopted from the SRKS model [1].

Table 4.3.: Matlab model general microstructural starting parameters

symbol	value	unit	description
A	350	[ ]	material specific constant
a_g	$2.87 \cdot 10^{-10}$	[m]	unit cell size
α	0.042	[ ]	constant for dislocation interaction
b	$2.87 \cdot 10^{-10}$	[m]	burgers vector
β	$6.00 \cdot 10^{7}$	[ ]	parameter to control the density of sources
c_{dip}	0.3	[ ]	weighting factor
d_{anh}	$5.90 \cdot 10^{-8}$	[m]	dislocation annihilation length
D_s	$3.88 \cdot 10^{-21}$	[m^2/s]	coefficient for self diffusion
D_{vp}	$5.01 \cdot 10^{-18}$	[m^2/s]	coefficient for pipe diffusion
η_v	0.02	[ ]	vacancies transfer coefficient
G	$6.20 \cdot 10^{10}$	[Pa]	shear modulus
h_b	$7.00 \cdot 10^{-8}$	[m]	spacing of dislocations within subgrain walls
M	3	[ ]	Taylor factor
ν	0.4	[ ]	Poisson's ratio
Q	$4.01 \cdot 10^{-19}$	[J]	activation energy
v_{cc}	$9.70 \cdot 10^{-14}$	[m/s]	dislocations constant climb velocity
Ω	$1.15 \cdot 10^{-29}$	[m^3]	atomic volume
Ω_{mult}	21.8	[ ]	dislocation movement displacement factor
W	$7.96 \cdot 10^{-19}$	[J]	pipe diffusion activation energy
ζ	0.55	[ ]	factor of influence of dislocation dipoles on boundary dislocations

The values in table 4.4 were used as the microstructural starting parameters for the individually mentioned calculations. For the corresponding creep curves and TTR-diagrams see chapter 5.3 starting on page 44.

Table 4.4.: Matlab model specific microstructural starting parameters

	unit	BM 650°C	MgC 600°C	Weld 600°C	Weld 625°C	Weld 575°C
ρ_b	[$1/m^2$]	$1.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$
ρ_{dip}	[$1/m^2$]	$1.50 \cdot 10^{13}$	$0.50 \cdot 10^{13}$	$0.50 \cdot 10^{13}$	$0.50 \cdot 10^{13}$	$0.50 \cdot 10^{13}$
ρ_m	[$1/m^2$]	$1.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$	$0.50 \cdot 10^{14}$
ρ_t	[$1/m^2$]	$3.15 \cdot 10^{14}$	$1.05 \cdot 10^{14}$	$1.05 \cdot 10^{14}$	$1.05 \cdot 10^{14}$	$1.05 \cdot 10^{14}$
R_{sg}	[$1/m^2$]	$0.25 \cdot 10^{-6}$	$1.00 \cdot 10^{-6}$	$1.00 \cdot 10^{-6}$	$1.00 \cdot 10^{-6}$	$1.00 \cdot 10^{-6}$
a_1	[$1/m^2$]	22.2	22.2	18.5	17.0	25.0

4.2. Microstructural analysis by EBSD

Electron backscatter diffraction (EBSD) is a method to study any (poly-)crystalline material. By making use of the Scanning Electron Microscope (SEM), this technique allows to understand the phase of materials, the structure and also the crystal orientation. In a modern lab, EBSD is conducted using a SEM equipped with an CMOS-camera behind a phosphor screen and allows indexing of the EBSD-patterns at up to 1800 patterns per second [68].

Prior to measuring in the SEM, the sample specimens as listed in chapter 4.1 had to be prepared. This task was thankfully performed by P. Garstenauer.

- Sawing with an 'Struers Accutom-10' equipped with an alumina disk type '40A15' at a cutting speed of 0.1 $^{mm}/_{s}$ with 3000 revolutions per minute of the cutting disk.
- Embedding in 'Polyfast' at 180°C in the 'Struers CitoPress-20'.
- Grinding in a 'Struers Tegramin-30' with SiC-foils at grit number #320 to #2000 in 5 stages, 3 minutes at 15 N. Followed by polishing for 15 minutes each with DiaDuo2 3 µm and 1 µm, rotation 40/90. Finishing with undiluted 'OP-S' for 30 seconds each with 30 N and 5 N, rotation 150/150.
- Final vibration polishing in the Buehler Vibromet 2, with 'OP-AN' for 20 hours.

The physical measurements in the SEM prior to the evaluation were taken by B. Krenmayr on a 'TESCAN Mira 3-XM' with an 'AMETEK Octane Super' EBSD-detector.

The measurements to determine the grain- and subgrain-structure span over a sample area of 40 x 40 µm with a step size of 50 nm. It has to be noted that a hexagonal scanning pattern was used, not a square-shaped one.

EBSD measurements to determine the size of the prior austenitic grains (PAGS) extended over an area of 500 x 500 µm with a hexagonal resolution of 600 nm.

Final evaluation of the data and creation of graphical maps was done in 'OIM Analysis v8.0'. The cleanup was performed with 'Grain CI Standardization' at a grain tolerance angle of 15 and a minimum grain size of 10. This is followed by a 'Neighbor CI Correlation' at a minimum confidence index of 0.75.

The grain- and subgrain sizes were determined by generating boundary maps first and then calculating them via automatic measurement in the software as well as manual counting of boundaries by means of the 'mean linear interface'-method after excluding all data under a confidence index of 0.70.

4.3. MatCalc thermodynamic calculations

Its developers describe MatCalc as a specialised 'scientific software toolbox' for computer simulation. Used in this thesis are its capabilities in calculation of constrained and unconstrained phase equilibria as well as multi-component and multi-phase precipitation kinetics. This is achieved by means of 1D and 2D long-range diffusion simulation and simultaneous precipitation calculations in addition to phase transformations. [69]

The CALPHAD-method and CALPHAD-type databases provide the necessary thermodynamic foundations, and are freely available in a limited version for Fe, Al- and Ni-based systems. Without a license, the MatCalc 6 software is limited to three simultaneous elements. [69, 70]

MatCalc is usually used with the assistance of its graphical user interface (GUI), because it's easy to understand and convenient to operate. Nevertheless, the ability to script all instructions has tremendous benefits: Every command is documented as a line of code, no typos or accidental misclicking which may lead to incomprehensible results because every result can be reviewed and reproduced. After changing anything (e.g. the chemical composition or other variables), only one simple rerun of the script is needed for a complete recalculation and graphical representation.

Part of the work of Schmid [1] is based on a precipitation kinetics script by Riedlsperger [12] for MatCalc 5.62. The rewriting of the script in native 6.01 language was done in this thesis because it offers several advantages: By making use of the new syntax, every reader can understand the code much easier because all code is written in full words and no longer in one-character abbreviations. In addition to that, the newest databases are not supported on the older version. Also, any new improvements in the underlying code and model of MatCalc will only be implemented in the newest branch.

The version used was MatCalc 6.01 (rel 1.003), released 2018-04-26. The free databases bundled with the installer are partly faulty, therefore the thermodynamic database mc_fe_v2.059.tdb (07/2016) and database for diffusion mc_fe_v2.011.ddb (10/2016) were downloaded from the homepage of the developers.

Sometimes the identical script on two different PC's may yield diverging results due to indeterminable reasons, especially regarding the Z-phase. For this thesis, the calculations were performed on these two systems and produced identical results: Windows 7 (64 Bit) on an Intel i7-4930k with 32 GB RAM and with Windows 10 (64 Bit) on an Intel i5-8250U with 8 GB RAM.

4.3.1. Equilibrium calculations

A 'Stepped Equilibrium script' is written to calculate the amount of occuring phase fractions and their chemical composition in equilibrium state. Shortly summarised, after initializing the workspace and loading all necessary databases, it reads the chemical composition of the alloy, includes all desired phases and then performs a stepwise calculation of all equilibrium states for a temperature range from 1600°C to 400°C in

temperature intervals of 10 K. A typical diagram as the result of this calculation can be seen in figure 5.5 on page 35.

The 18 elements included are: Fe, Si, Mn, Cr, Ni, Mo, V, Nb, W, Cu, Ti, Al, Co, P, B, N, S, C and vacancies.

The phases (MatCalc nomenclature) comprise of: LIQUID, FCC_A1, BCC_A2, M23C6, LAVES_PHASE, SIGMA, ALN, BN_HP4, M2B, CU2S, ZET and ALN_EQU.

Additional custom phases were created to differentiate between different compositions of MX-phases with the following major constituents: NbC, VN and TiN. It is very important to define the custom composition phases correctly, otherwise MatCalc will give a warning to check the results due to 'inconsistent major constituents' and the calculation will even cancel because of 'too many iterations'.

The script is located in the appendix of this thesis ranging from page 70 to page 73. It is a combined script which also performs the 'Scheil-Gulliver'-calculations described in the next subchapter.

Furthermore (by the means of an additional script provided on the enclosed DVD, but not printed in the appendix due to its length), detailed plots of the contents of all phases or the distribution of desired specific elements can be plotted, for example the composition of chromium carbides (Figure 5.6 on page 36) or the distribution of chromium itself in all phases (figure 5.7 on page 36).

4.3.2. Scheil-Gulliver

The second script created is a 'Scheil-Gulliver' calculation. It simulates the segregation of elements during the solidification of a system. The segregation of elements is of particular interest to calculate the average chemical composition of the materials' matrix (which will affect the precipitation simulations later on) originating from the bulk chemical analysis.

The script is also part of the Equilibrium script in the appendix of this thesis, ranging from page 70 to page 73. Backdiffusion from C,B,P,N & S is considered as well as the possible peritectic phase transformation from BCC to FFC-iron (figure 5.8 on page 37). Starting temperature is set at 1525°C and the cooling step size is 1 K down to until 3% or 1% residual melt are reached, where 1% equals to a slower cooling process than 3%.

The numerical values gained from the calculated residual melt composition (graphical interpretation in figure 5.9 on page 37) are used to determine the main matrix composition after full solidification. This is done by the help of a small additional Excel-Sheet (see table 5.1 on page 38).

The resulting data is now the final input needed for the precipitation kinetics script introduced in the next subchapter.

4.3.3. Precipitation kinetics simulation

The precipitation kinetics simulation predicts the temporal evolution of the precipitates during all heat treatments and service time. All numerically generated data is stored for export to Matlab later. Additionally, diagrams which show the number density, phase fraction and the mean diameter of all precipitates during all heat treatments and service life are plotted.

The complete script with all settings and values used is located in the appendix, ranging from page 74 to page 106.

The coded thermal treatments encompass routines for austenizing, quenching, tempering, welding, PWHT and service time. All of them are implemented in the script, but only the latter three are utilised for this thesis (Figures 4.1 to 4.3).

After welding with an t8/5-value of 20 s and further cooling to room temperature, the material undergoes a post weld heat treatment. The PWHT is 4 hours holding at 760°C with heating and cooling rates of 80 K per hour. The desired service temperature is queried from the user after the script starts.

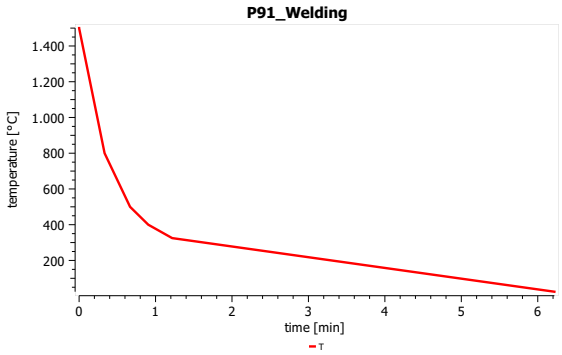

Figure 4.1.: Temperature curve for welding

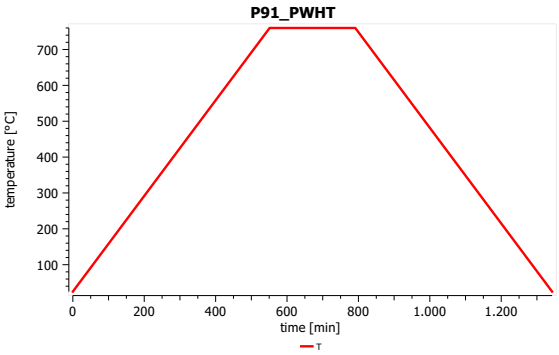

Figure 4.2.: Temperature curve for PWHT

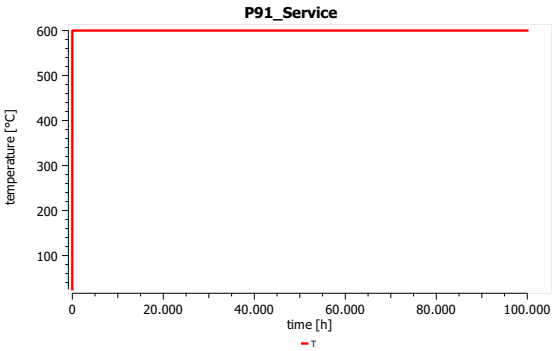

Figure 4.3.: Temperature curve for service

For the final export of the numerical results to Matlab, the values are copied manually with use of the MatCalc GUI. This happens with an right click on the corresponding

service diagram of the number density (e.g. figure 5.18 on page 43) or the mean diameter (e.g. figure 5.17 on page 42). Then, in the appearing context menu, 'Copy to clipboard/Plot/Data' is selected.

Figure 4.4 shows a small excerpt of such an excel sheet, where the 'auto' value corresponds to the time passed [h] and the second value to the mean diameter [µm].

auto	NbC(mart,d)	auto	NbC(mart,g)	auto	NbC(mart,s)	auto	VN(aust,d)	auto	VN(aust,g)
10,068	14,05488	10,068	50,12785	10,068	14,05490	10,068	21,88254	10,068	215,80977
10,305	14,05478	10,305	50,12191	10,305	14,05479	10,305	21,87869	10,305	215,66490
10,514	14,05469	10,514	50,11656	10,514	14,05470	10,514	21,87455	10,514	215,45806
10,747	14,05458	10,747	50,11038	10,747	14,05460	10,747	21,86963	10,747	215,76206
10,963	14,05449	10,963	50,10450	10,963	14,05451	10,963	21,86629	10,963	215,13022
11,184	14,05439	11,184	50,09829	11,184	14,05441	11,184	21,86246	11,184	214,92740
11,411	14,05429	11,411	50,09172	11,411	14,05431	11,411	21,85740	11,411	215,16806
11,649	14,05419	11,649	50,08455	11,649	14,05421	11,649	21,85324	11,649	214,78284
11,885	14,05409	11,885	50,07718	11,885	14,05410	11,885	21,85036	11,885	214,73093
12,181	14,05396	12,181	50,06745	12,181	14,05397	12,181	21,84728	12,181	214,11036

Figure 4.4.: Example for mean diameter MatCalc data export

As mentionend, a kinetics script by Riedlsperger [12] written for MatCalc 5.62 already existed, but the translation and transfer into 6.01 has raised some issues. All important adjustments and settings listed here to circumvent these problems are also valid for the other MatCalc-scripts where applicable.

In addition to the faulty databases bundled with the installer of version 6.01, one additional important bug was found in this current version which is of great importance for the precipitation kinetics simulation: Usually a 'subgrain elongation factor' is set for the martensitic precipitation domain corresponding to the martensite lath shape. Unfortunately, if this variable is set to any other value than '1', MatCalc sets it to 'zero' and absolutely no precipitates occur on any subgrain boundaries because no valid nucleation sites are available.

It is important to work with high enough number of precipitate size classes, a value of 50 has turned out to be adequate for reliable results. A number of e.g. 25 classes gives results much faster, but is unreliable especially for Z-phase evolution.

One other critical matter to bear in mind is the verification of the composition of all phases during the simulation. If the option to enforce the major constituents is not set (especially for the MX-phases), it can happen, that e.g. all VN-phases are in reality mostly consisting of Niobium and Carbon or vice versa. This would lead to further problems later, because the nucleation of the modified Z-phase is bound to the vanadium nitrides in the code.

4.4. Matlab creep modelling

For the numerical implementation of the creep model, all formulas are embedded in Matlab as the development environment. It also provides the framework for an easy to use GUI and all tools for input of data and output of results as well as creation of graphics and diagrams. The MATLAB version used was 2018a with update 6 applied.

According to the developers, MATLAB is an extensive and sophisticated development environment and programming language for solving mathematical problems and has application in image, signal and data analysis. The name derives from the term "MATrix LABoratory", a hint that MATLAB is optimised to operate on arrays and whole matrices. Consequently, the variables used are treated as multidimensional arrays, regardless of the data type. The internal calculation precision is by standard 64 Bit floating point (base 2) according to IEEE754. [71]

4.4.1. Modifications to preliminary existing code

The code as received from Schmid [1] was extensively reworked and enhanced. This includes many small changes like implementing new experimental creep data from literature [9], adding comments to the code, coding a progress bar and automated labelling on all diagrams.

To allow the implementation of an automatic TTR-curve calculation via loops, great parts of the code had to be reorganised into a different file structure. This was also a prerequisite for making it possible for several users to work on the software at the same time without the need to delete older precipitation data, creep curves or settings. It also allowed another small speedup by about 10 seconds per creep curve after the first one because all excel files now have to be only read once.

Simultaneously, the file names were unified and shortened. Figure 4.5 shows all files of the Matlab-model.

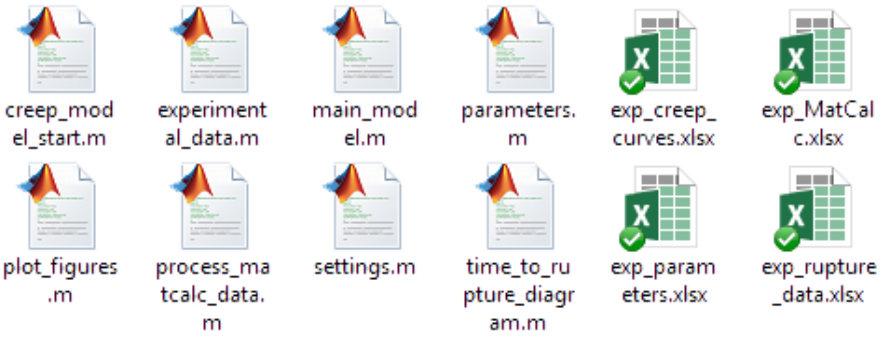

Figure 4.5.: Matlab model files

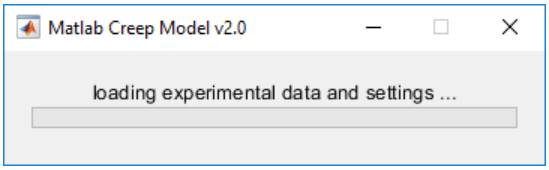

Figure 4.6.: Progress bar loading parameters

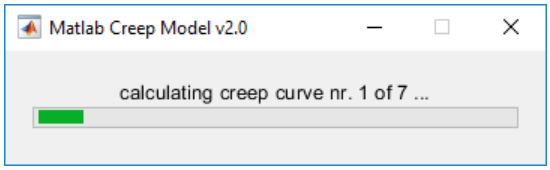

Figure 4.7.: Progress bar calculating creep

creep_model_start.m - This is the main framework file that starts the model. It is responsible for preloading all data which does not change over several loops as well as calling all other scripts when needed. This includes fit-parameters and microstructural data from **exp_parameters.xlxs**. It also creates the newly generated calculation progress bars (see figure 4.6 and 4.7).

settings.m - Here the input dialogue (figure 4.9) is created and defined as well as prefilled with standard selections. All these choices are of fundamental importance for the creep model and will also determine from which excel-tabs experimental data will be fetched later.

experimental_data.m - This script loads the experimentally determined creep curves from **exp_creep_curves.xlxs** as well as the TTR-curves from **exp_rupture_data.xlxs** for later plotting and comparing to the calculated results.

process_matcalc_data.m - The results from the MatCalc precipitation kinetic simulation are here loaded from **exp_MatCalc.xlxs** and elaborately reorganised for further use in the model.

parameters.m - Here all preloaded strings from the parameters excel-file are split up and assigned to single variables.

main_model.m - All the governing equations are located here, the greatest part of this file is looped for as long as one of the stop criteria is fulfilled (for example 10^5 hours of service or over 6% elongation).

plot_figures.m - Here the simulated creep curve is plotted in a diagram to be able to compare its shape with an experimentally determined creep curve (e.g. figure 5.19 on page 44).

time_to_rupture_diagram.m - In this final Matlab file, after all calculations are finished, the time-to-rupture diagram is created. Here the simulated rupture points can easily be compared to all included experimental rupture data (e.g. figure 5.22 on page 45).

Figure 4.8 on the left side shows the old input mask by Schmid [1]. Here a lot of microstructural data and fit-parameters were to be entered directly. The applied stress and temperature were not decoupled from the experimental datasets, only data for 80 MPa and 100 MPa at 650°C was available.

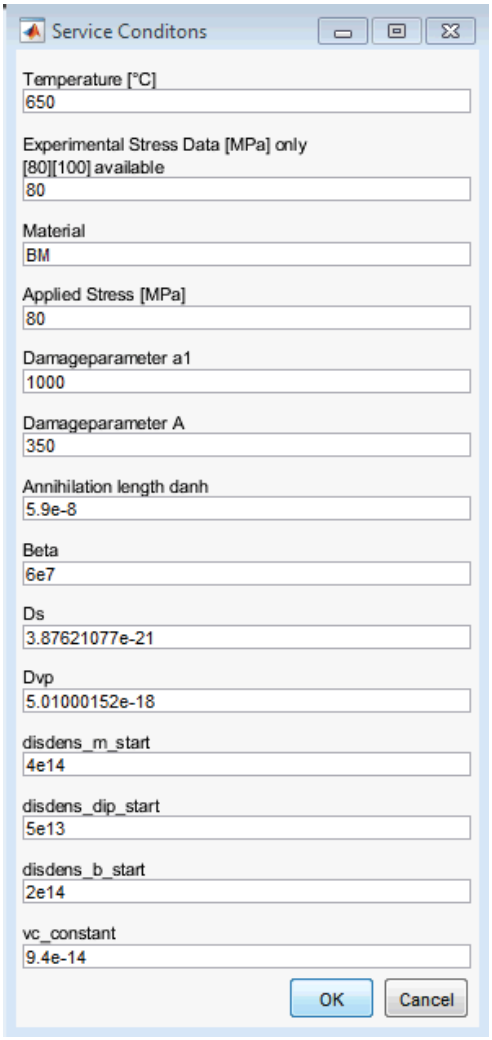

Figure 4.8.: Old Matlab model GUI

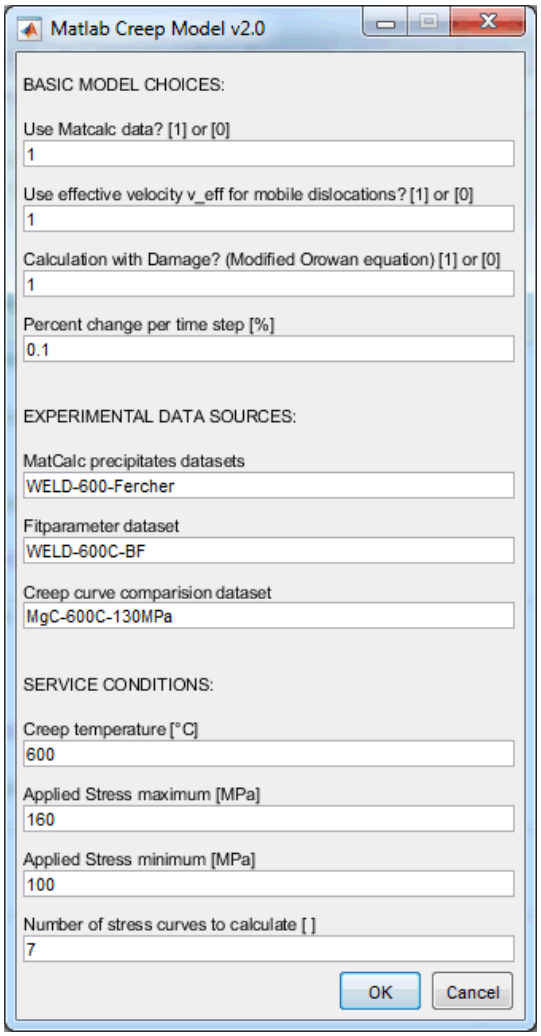

Figure 4.9.: New Matlab model GUI

As can be seen in figure 4.9, the new mask and the underlying code changes offer now several powerful features. In the dialogue, [1] corresponds to 'yes' while [0] means 'no'. The service conditions can be chosen independently from the experimental data sources. These sources are cumulated in separate tabs in the mentioned excel files and can be chosen freely from.

As a result, it is now possible to e.g. calculate a creep curve at 650°C with data and fit-paramaters aquired at 600°C and compare it to a suitable dataset.

The last three input lines define the upper and lower limit for the applied stresses and the number of curves to calculate. They will be evenly distributed over the specified range by the script.

5. Results

In this chapter the results of the present work are listed and graphically illustrated. Interpretation of all the results is carried out in chapter 6. To make them more accessible, the results have been again divided into individual subchapters for the microstructural analysis, Matcalc and Matlab.

5.1. EBSD microstructural data

The EBSD analysis of one piece of unaltered weld material (internal reference: 'BOA 1', see also chapter 4.1, table 4.1 on page 23) yields following results, which were needed for the precipitation kinetics simulation and the creep model.

Figure 5.1 shows the generated grainmap with a scan size of 40 x 40 µm with a scanning step size of 50 nm. The colours illustrate the crystallographic orientation while the gray borders correspond to the image quality for each pixel.

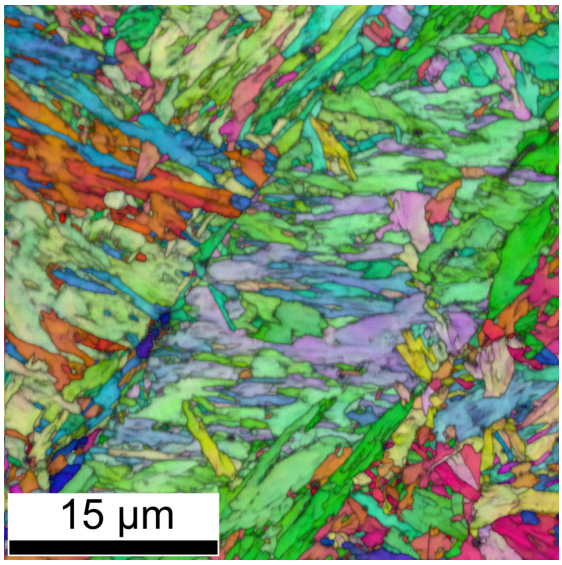

Figure 5.1.: Grainmap inverse pole figure + IQ

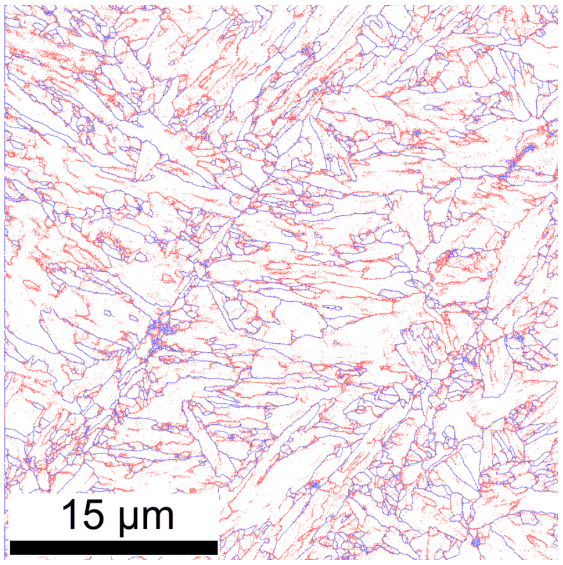

Figure 5.2.: Grainmap borders LAGB and HAGB

Figure 5.2 represents the same dataset. The blue lines correspond to the high angle grain boundaries (misorientation angle >15°), the red lines to the low angle grain boundaries (misorientation angle <15°).

Here grains are defined as structures surrounded by high angle grain boundaries (blue), while subgrains are additionally confined by low angle grain boundaries (red).

Assessed with the automatic functions of OIM Analysis 8.0, the average grain diameter is determined at 8.04 µm, the average subgrain diameter 4.09 µm. The manual counting of grain boundaries via mean interception method gives a much lower value for subgrain sizes in the range of 1 µm diameter.

The wider scan for the determination of the prior austenitic grain size is illustrated in figures 5.3 and 5.4. It extends over an area of 500 x 500 µm with a hexagonal resolution of 600 nm.

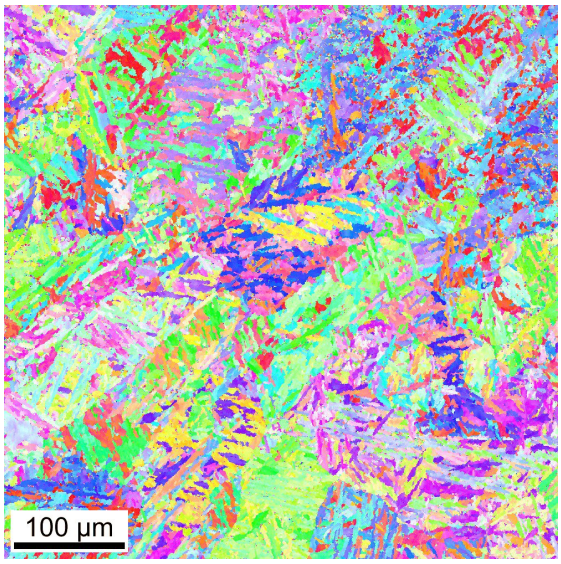

Figure 5.3.: PAGB: Grainmap inverse pole figure

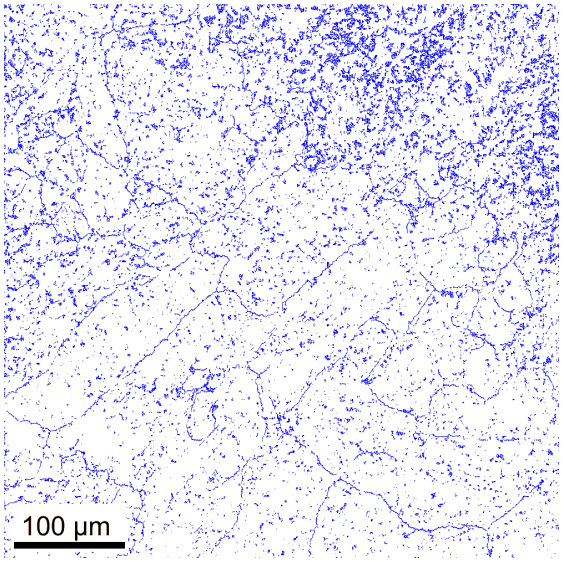

Figure 5.4.: PAGB: Grainmap borders for 20 to 50° misorientation angle

The evaluation of the borders with a local misorientation angle of 20-50° in figure 5.4 leads to an estimated PAGS of about 50-75 µm. It was not achievable to get a picture with more usable information or clearer borders by varying the upper or lower misorientation angle limits.

5.2. MatCalc

Representative MatCalc diagrams for all simulations done will be presented and shortly described here, but not discussed contentwise.

5.2.1. Equilibrium calculations

Figure 5.5 shows the graphical representation of the numerical results from the stepped equilibrium calculation for the bulk composition of the weld material (see first column in figure 5.1 on page 38).

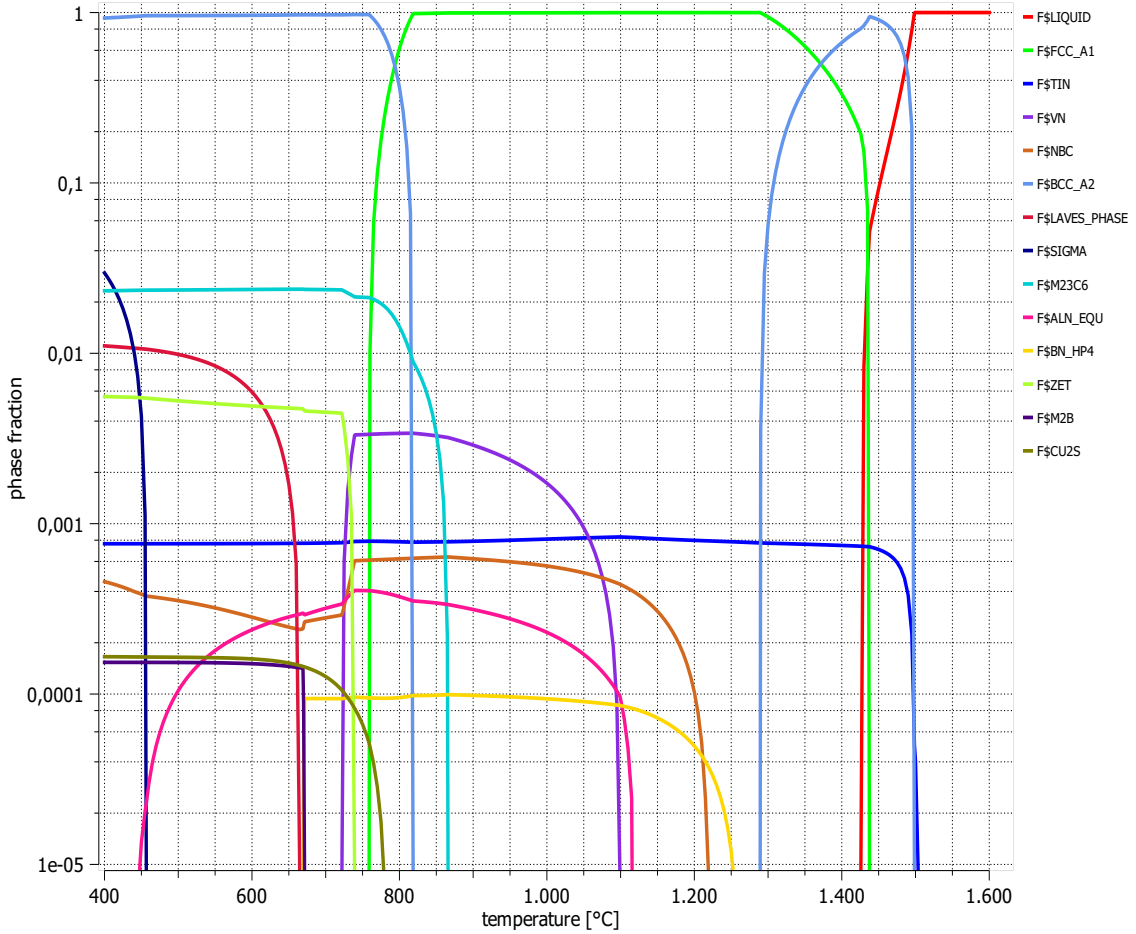

Figure 5.5.: Stepped equilibrium overview calculation

The vertical axis is scaled logarithmically for a better graphical interpretation of the curves, this applies to all Equilibrium and Scheil-Gulliver diagrams. The colour-coded legend is always on the right hand side.

Figure 5.6 shows the equilibrium composition of $M_{23}C_6$ for one mole of system.

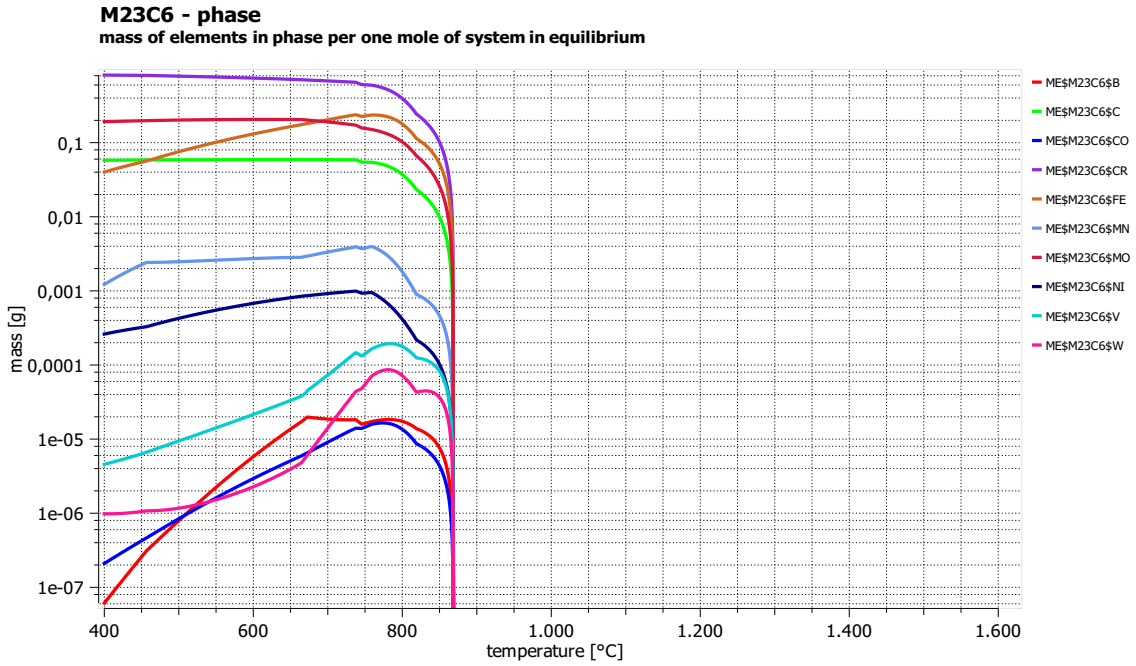

Figure 5.6.: Equilibrium phase composition for $M_{23}C_6$

Figure 5.7 illustrates the distribution of chromium in one mole of system in equilibrium.

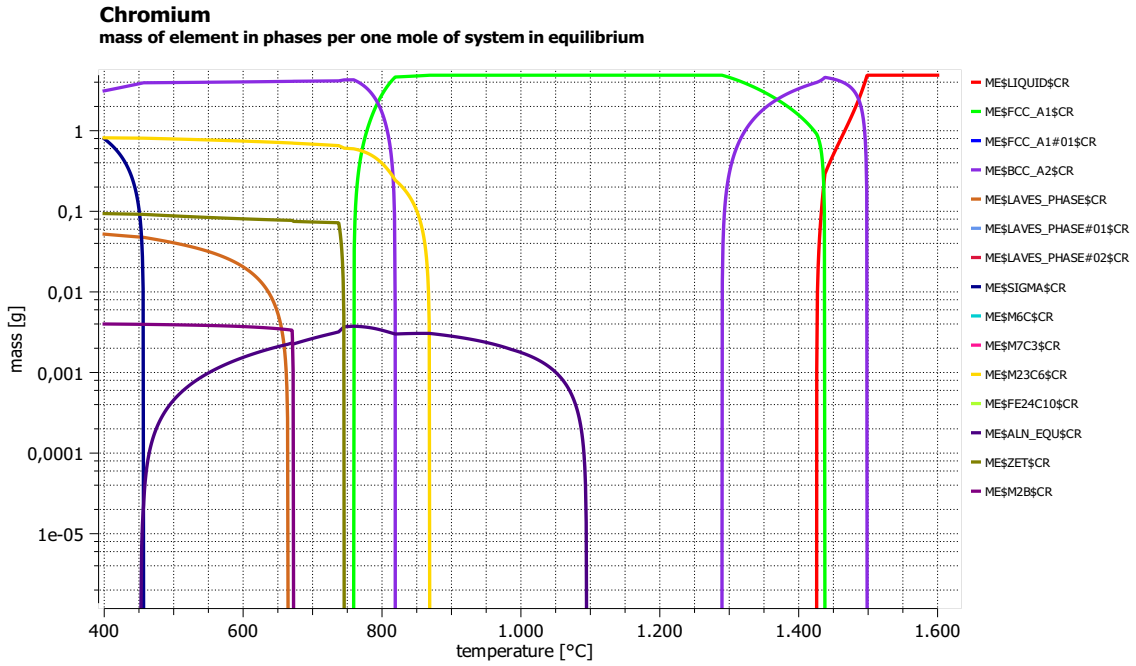

Figure 5.7.: Equilibrium phase distribution of Cr

5.2.2. Scheil-Gulliver

Figure 5.8 displays the phase composition in disequilibrium during solidification until 1% melt is left. The violet phase is FCC-iron created by peritectic transformation.

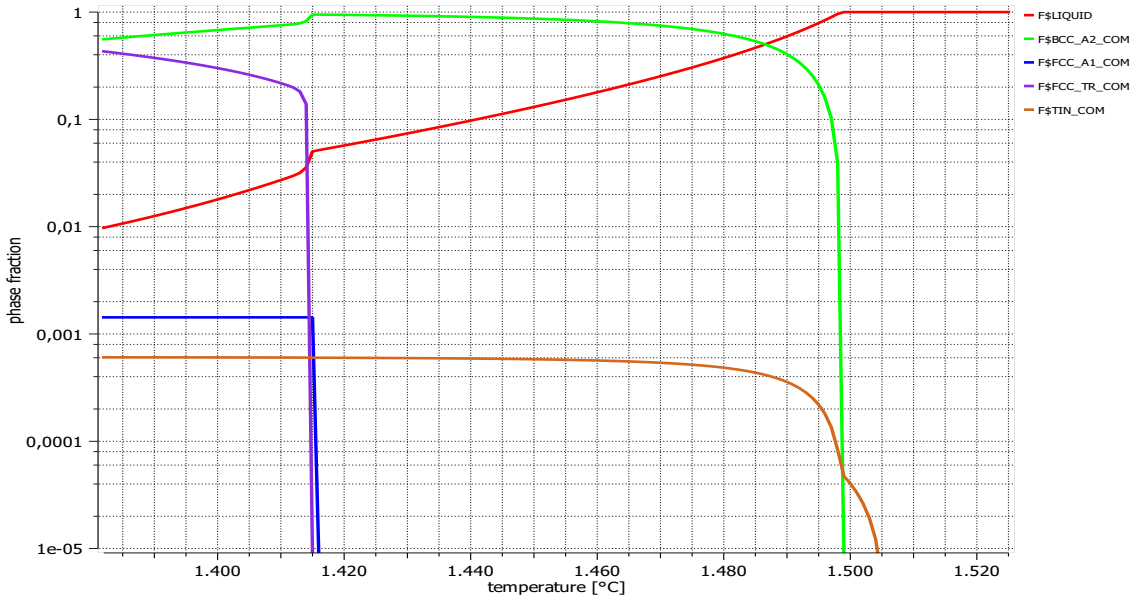

Figure 5.8.: Phase composition in disequilibrium during solidification

Figure 5.9 demonstrates the enrichment and depletion of elements in disequilibrium for one mole of system during solidification of the melt.

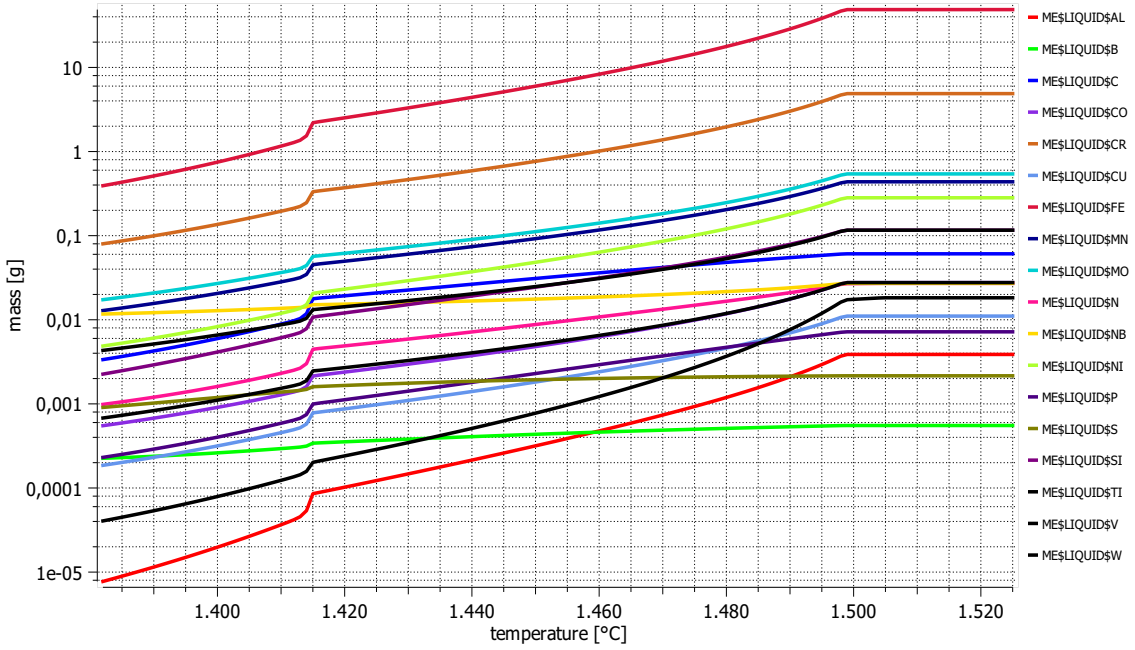

Figure 5.9.: Enrichment and depletion of elements in disequilibrium during solidification

After performing the Scheil-Gulliver solidification simulations, the chemical composition of the residual melt is entered into second column-group of the excel table as seen in table 5.1.

	chemical analysis 1 fraction		1% residual melt 0,009812 fraction		matrix 0,990188 fraction		matrix normalized 1 fraction		enrichment in melt	depletion in matrix	
	wt-fraction	weight-%	wt-fraction	weight-%	wt-fraction	weight-%	wt-fraction	weight-%	[%]	[%]	
Fe	8,81E-01	88,084%	7,36E-01	73,648%	8,74E-01	87,361%	8,82E-01	88,227%	-16,4%	0,16%	Fe
Cr	8,83E-02	8,830%	1,50E-01	14,998%	8,68E-02	8,683%	8,77E-02	8,769%	69,9%	-0,69%	Cr
Mn	7,90E-03	0,790%	2,41E-02	2,414%	7,66E-03	0,766%	7,74E-03	0,774%	205,6%	-2,04%	Mn
Mo	9,80E-03	0,980%	3,25E-02	3,255%	9,48E-03	0,948%	9,57E-03	0,957%	232,1%	-2,30%	Mo
C	1,10E-03	0,110%	6,33E-03	0,633%	1,04E-03	0,104%	1,05E-03	0,105%	475,7%	-4,71%	C
Ni	5,10E-03	0,510%	9,14E-03	0,914%	5,01E-03	0,501%	5,06E-03	0,506%	79,2%	-0,78%	Ni
Si	2,10E-03	0,210%	4,23E-03	0,423%	2,06E-03	0,206%	2,08E-03	0,208%	101,5%	-1,01%	Si
V	2,10E-03	0,210%	8,13E-03	0,813%	2,02E-03	0,202%	2,04E-03	0,204%	287,1%	-2,85%	V
N	4,90E-04	0,049%	1,83E-03	0,183%	4,72E-04	0,047%	4,77E-04	0,048%	273,0%	-2,70%	N
Co	5,00E-04	0,050%	1,03E-03	0,103%	4,90E-04	0,049%	4,95E-04	0,049%	106,6%	-1,06%	Co
Ti	3,30E-04	0,033%	8,49E-05	0,008%	3,29E-04	0,033%	3,32E-04	0,033%	-74,3%	0,74%	Ti
Nb	4,90E-04	0,049%	2,19E-02	2,188%	2,75E-04	0,028%	2,78E-04	0,028%	4365,5%	-43,26%	Nb
P	1,30E-04	0,013%	4,34E-04	0,043%	1,26E-04	0,013%	1,27E-04	0,013%	233,6%	-2,32%	P
Cu	2,00E-04	0,020%	3,49E-04	0,035%	1,97E-04	0,020%	1,99E-04	0,020%	74,4%	-0,74%	Cu
W	5,00E-04	0,050%	1,28E-03	0,128%	4,87E-04	0,049%	4,92E-04	0,049%	155,0%	-1,54%	W
Al	7,00E-05	0,007%	1,45E-05	0,001%	6,99E-05	0,007%	7,05E-05	0,007%	-79,3%	0,79%	Al
S	3,90E-05	0,004%	1,70E-03	0,170%	2,23E-05	0,002%	2,25E-05	0,002%	4261,6%	-42,23%	S
B	1,00E-05	0,001%	4,23E-04	0,042%	5,85E-06	0,001%	5,91E-06	0,0006%	4130,8%	-40,93%	B

Table 5.1.: Matrix composition calculation table after Scheil-Gulliver

By combining both the original bulk composition (first column-group) and the composition of the residual melt with respect to the precise fraction at this composition it is possible to calculate the normalised matrix composition needed for the precipitation kinetics simulation.

The factor of enrichment or depletion in the matrix or the melt for each element is plotted in the last two columns.

5.2.3. Precipitation kinetics simulation

The diagrams for welding and PWHT are the same for all service temperatures. All additional figures regarding phase fraction, mean diameter and number density for all service temperatures are placed in the appendix, starting with table C.1 on page 130.

Figure 5.10 shows the evolution of the phase fractions during welding.

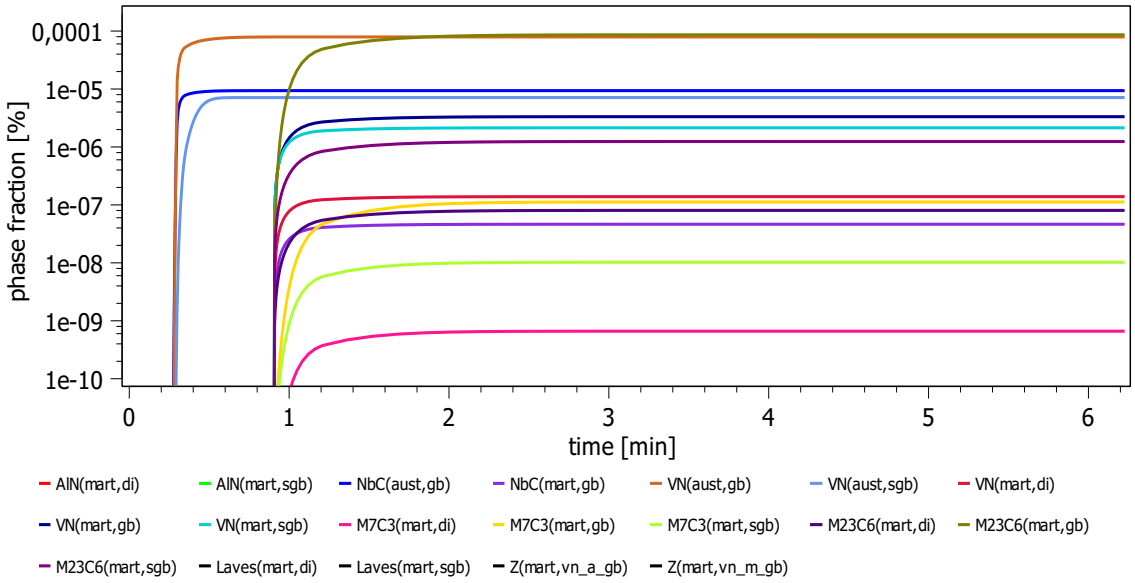

Figure 5.10.: Welding: phase fraction diagram

Figure 5.11 shows the evolution of the mean diameter during welding.

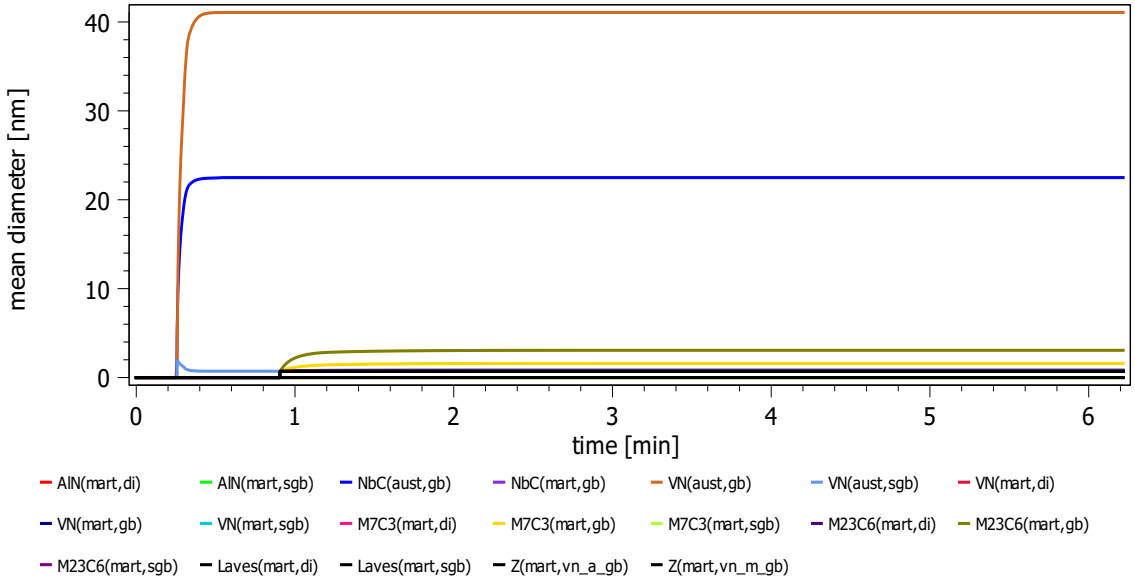

Figure 5.11.: Welding: mean diameter diagram

Figure 5.12 shows the evolution of the number density during welding.

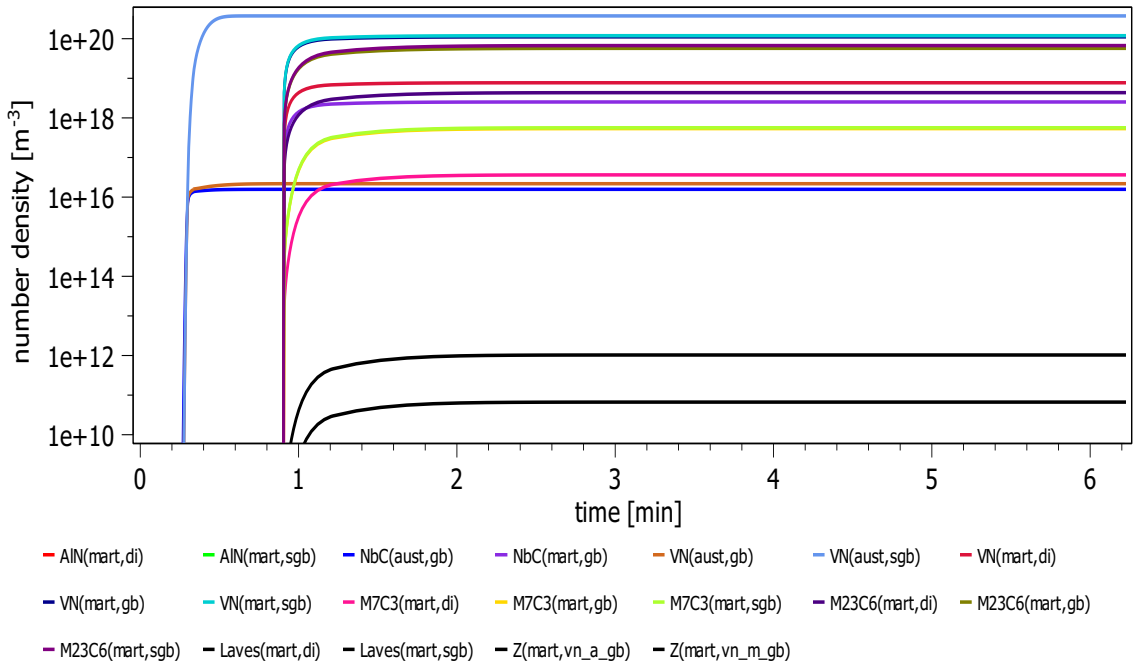

Figure 5.12.: Welding: number density diagram

Figure 5.13 shows the evolution of the phase fractions during PWHT.

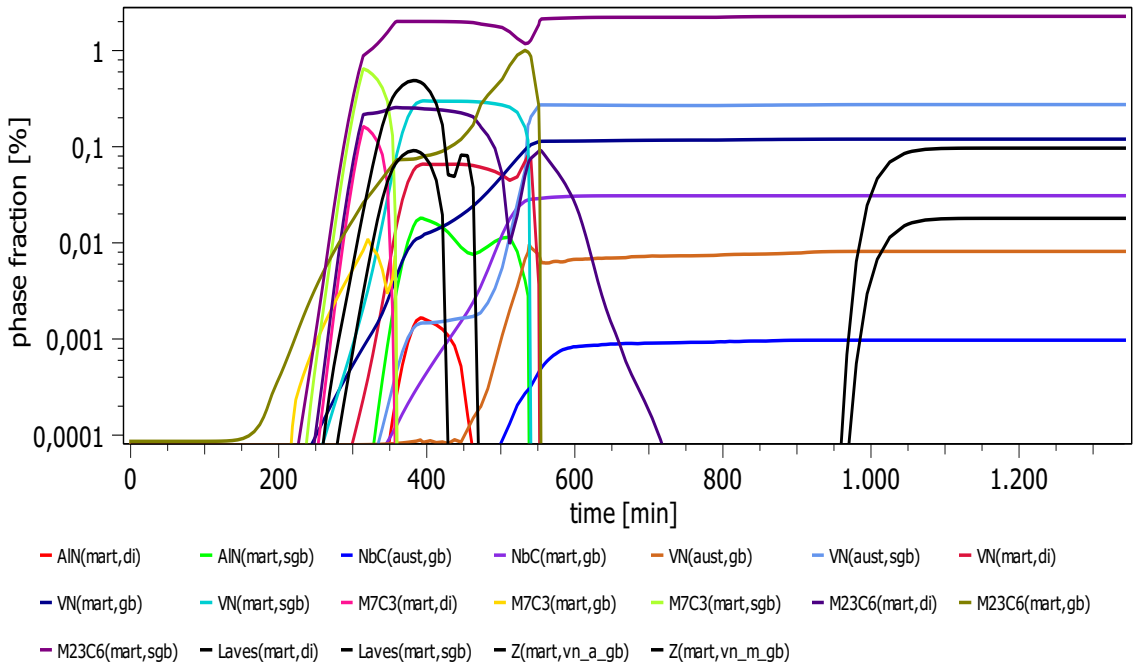

Figure 5.13.: Post weld heat treatment: phase fraction diagram

Figure 5.14 shows the evolution of the mean diameter during PWHT.

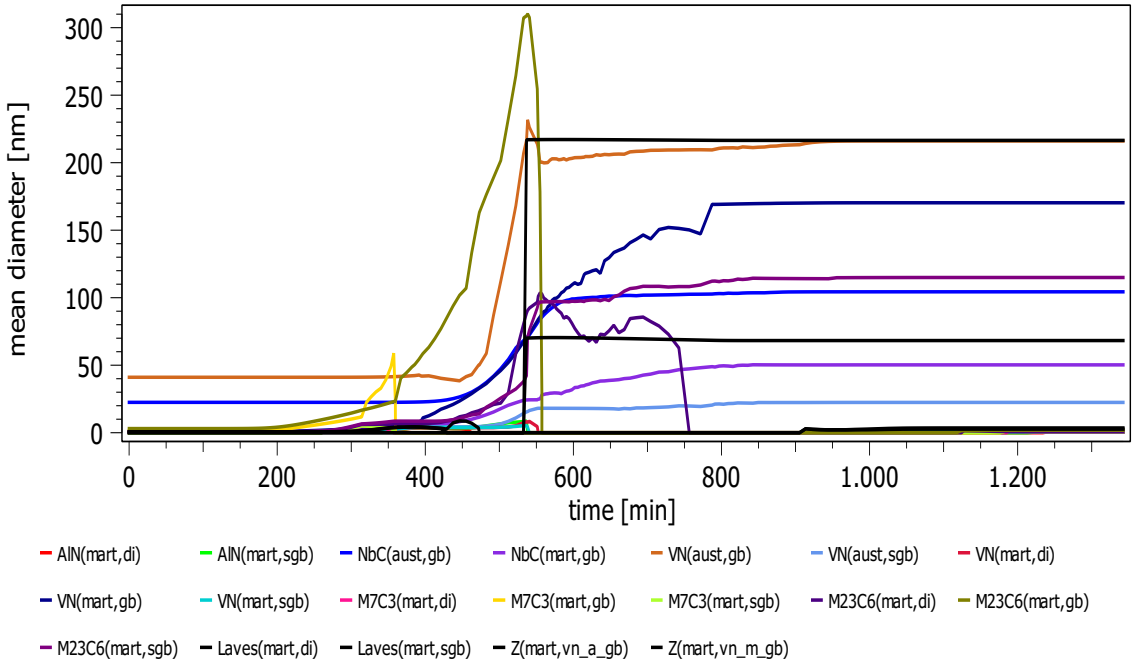

Figure 5.14.: Post weld heat treatment: mean diameter diagram

Figure 5.15 shows the evolution of the number density during PWHT.

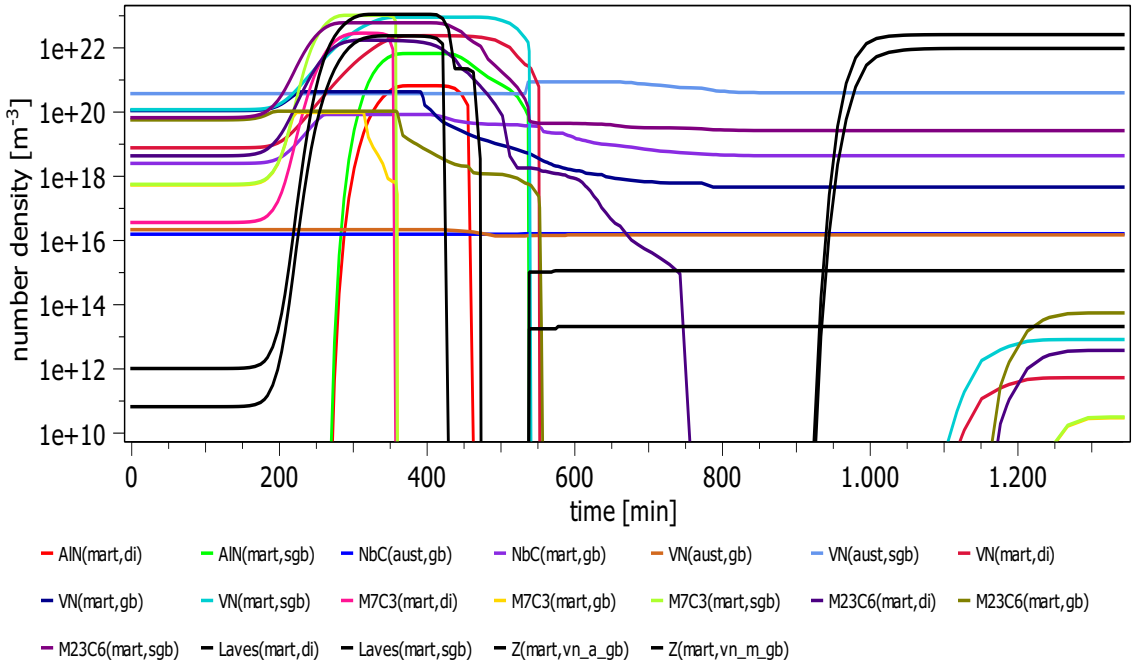

Figure 5.15.: Post weld heat treatment: number density diagram

Figure 5.16 shows the evolution of the phase fractions during service at 600°C.

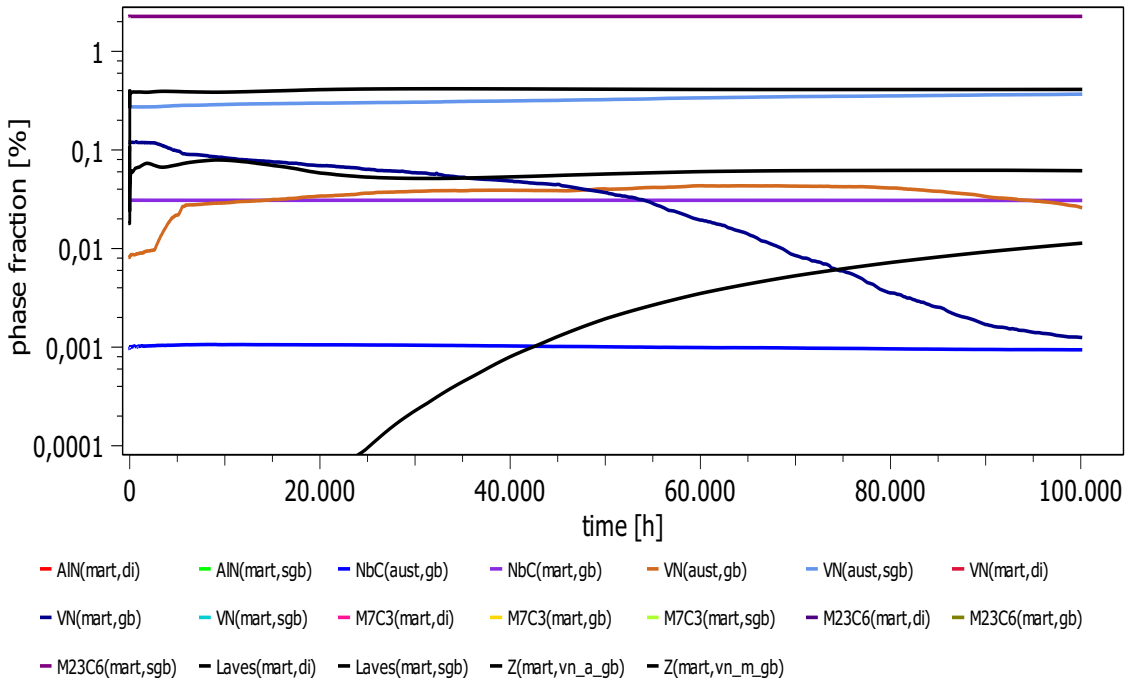

Figure 5.16.: 600°C service: phase fraction diagram

Figure 5.17 shows the evolution of the mean diameter during service at 600°C.

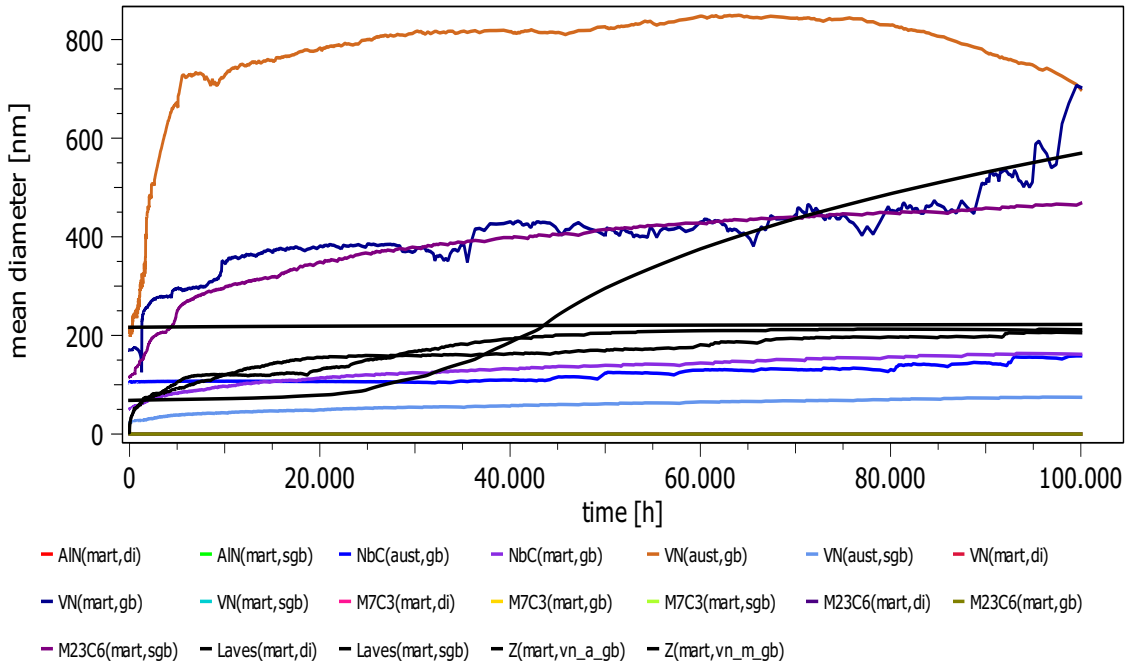

Figure 5.17.: 600°C service: mean diameter diagram

Figure 5.18 shows the evolution of the number density during service at 600°C.

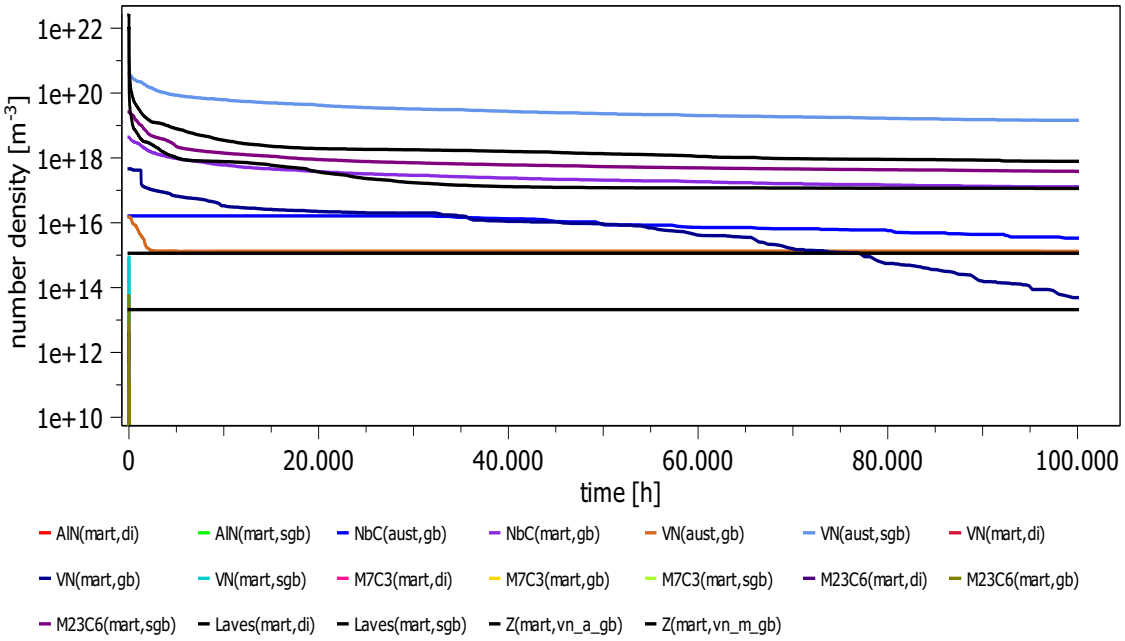

Figure 5.18.: 600°C service: number density diagram

Table 5.2 shows the numerical values of the precipitates' status at three points of service time at 600°C.

	phase fraction [%]			mean diameter [nm]			number density [m^{-3}]		
service at 600°C	**1000 h**	**10 000 h**	**100 000 h**	**1000 h**	**10 000 h**	**100 000 h**	**1000 h**	**10 000 h**	**100 000 h**
M23C6 (mart,sgb)	2,262	2,262	2,262	142	298	468	1,22E+19	1,41E+18	3,84E+17
Laves (mart,sgb)	0,387	0,386	0,411	57,7	120	205	3,31E+19	3,47E+18	7,86E+17
Laves (mart,di)	0,067	0,079	0,062	60,3	121	211	4,91E+18	7,68E+17	1,15E+17
VN (aust,gb)	0,009	0,029	0,026	259	729	699	5,84E+15	1,33E+15	1,31E+15
VN (aust,sgb)	0,273	0,290	0,368	27,1	43,0	74,5	2,31E+20	6,25E+19	1,44E+19
VN (mart,gb)	0,119	0,083	0,001	167	346	703	4,20E+17	3,34E+16	4,91E+13
NbC (aust,gb)	0,001	0,001	0,001	106	107	158	1,63E+16	1,63E+16	3,36E+15
NbC (mart,gb)	0,031	0,031	0,031	58,5	96,7	162	2,76E+18	6,06E+17	1,29E+17
mod. Z (aust,gb)	0,000	0,000	0,000	217	218	222	2,09E+13	2,09E+13	2,09E+13
mod. Z (mart,gb)	0,000	0,000	0,011	68,7	71,7	569	1,15E+15	1,15E+15	1,15E+15

Table 5.2.: 600°C service: phase properties

The tables and diagrams for mean diameter, number density and phase fraction for all other simulated service temperatures can be found in the appendix:

550°C: Table C.1 on page 130
575°C: Table C.2 on page 132
625°C: Table C.4 on page 136
650°C: Table C.5 on page 138

5.3. Matlab creep modelling

This section contains the collection of all important creep curves and TTR-diagrams from the Matlab creep simulation that will be the basis of discussion in chapter 6.

All model parameters and all values needed for the start microstructure are listed in tables 4.3 and 4.4 in chapter 4.1 on page 24.

Figure 5.19 shows the first new fit with all the new code and formulas with the original microstructural data from Schmid [1] at 650°C and 80 MPa.

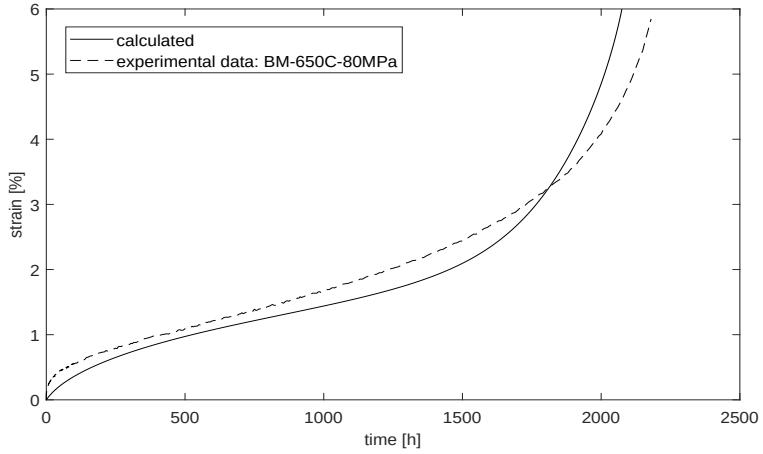

Figure 5.19.: Creep curve: New fit at 80 Mpa and 650°C with microstructural data from Schmid

Figure 5.20 compares the new TTR-curve and the original one from Schmid [1].

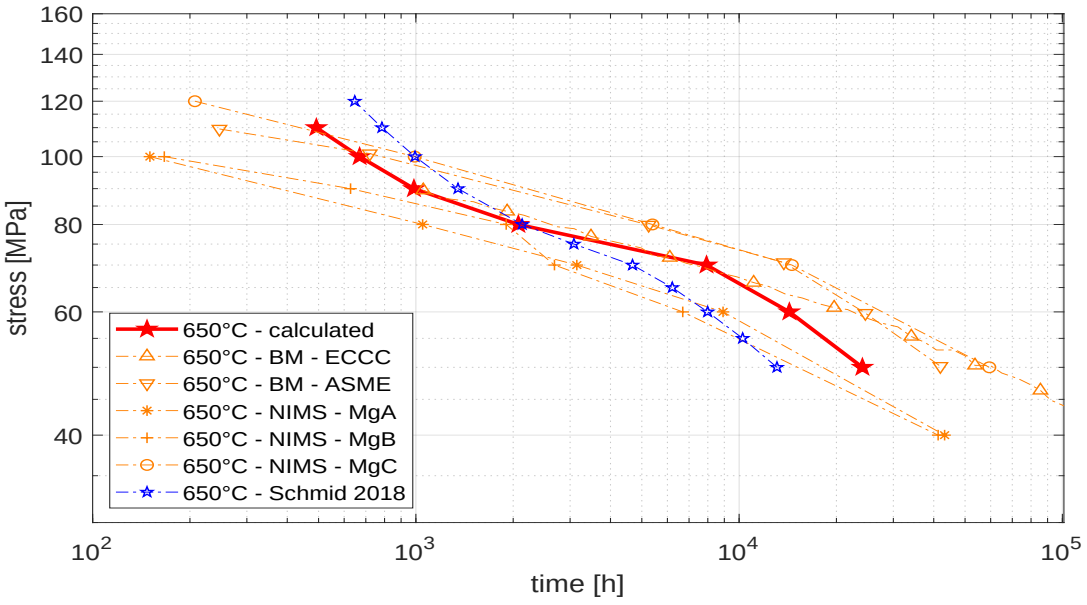

Figure 5.20.: Comparison of TTR-curves of Schmid and the new model at 80 Mpa and 650°C

Figure 5.21 illustrates the fitting of the creep curve at 600°C and 130 MPa with the weld microstructure. The reference creep curve derives from P91 experimental creep data by NIMS [9].

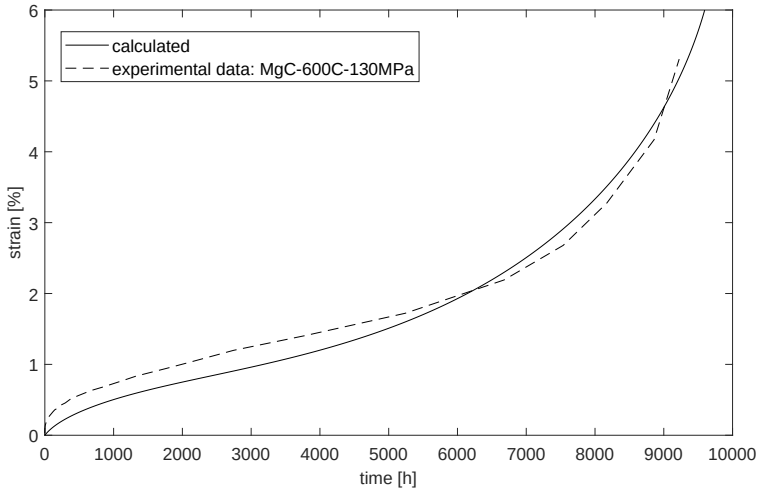

Figure 5.21.: Creep curve: Fit at 600°C and 130 MPa with own microstructural data

Figure 5.22 compares the simulated TTR-curve at 600°C with the experimental P91 creep rupture data from NIMS [9].

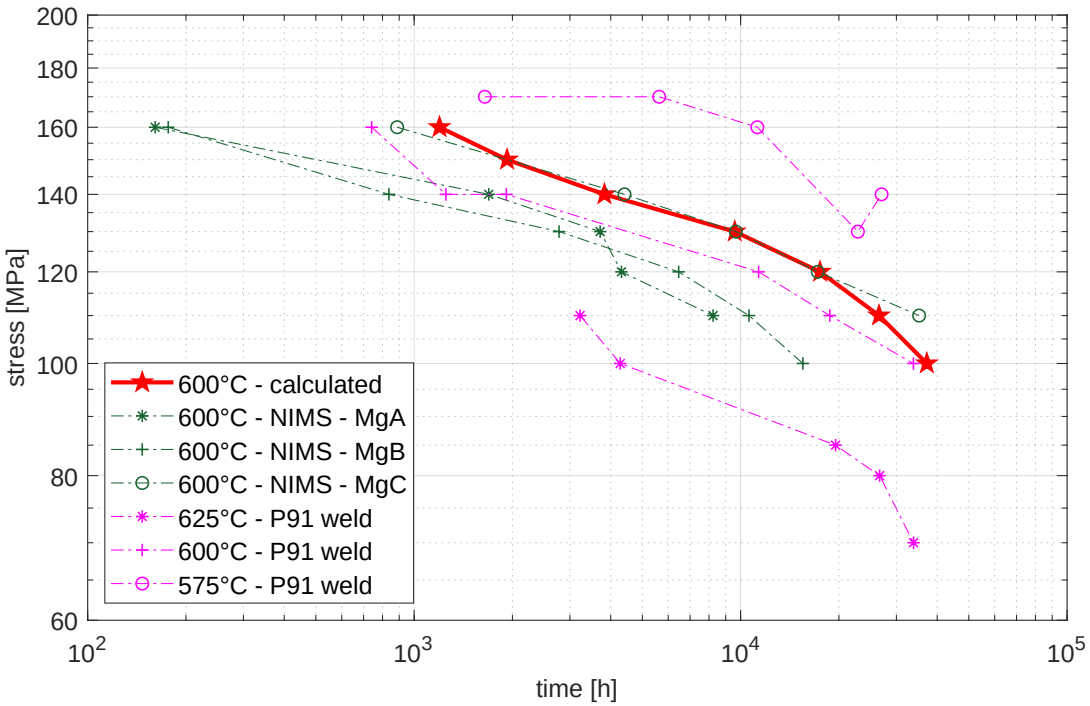

Figure 5.22.: TTR-diagram at 600°C with NIMS-reference and varying applied stresses

Figure 5.23 compares the simulated TTR-curve at 600°C with the experimental creep rupture data for P91 weld material from Böhler. The only variations regarding input data compared to figure 5.22 is the variation of the prefactor a_1 from 22 to 18.5.

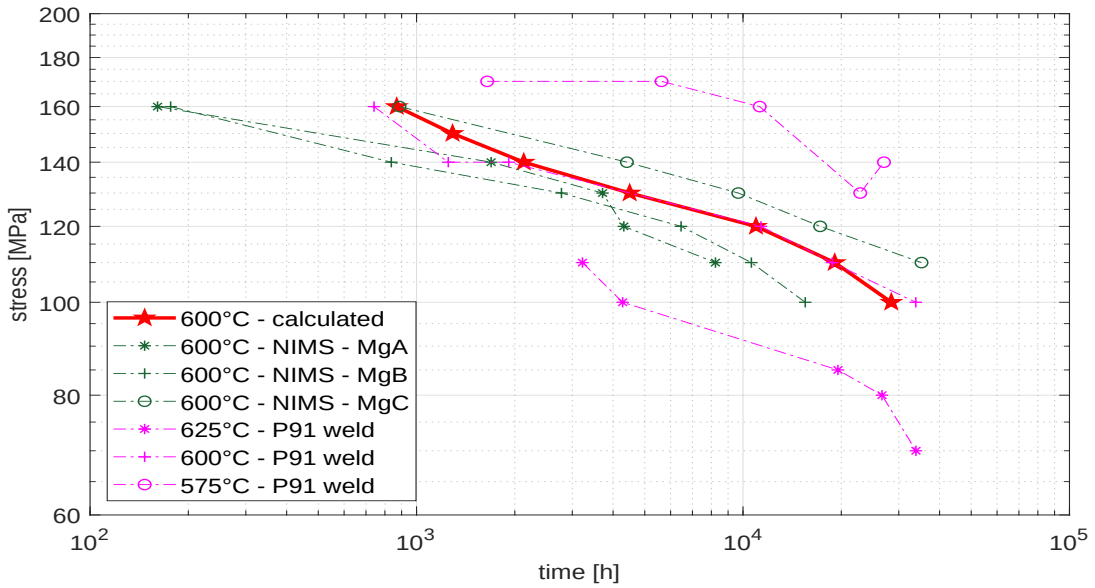

Figure 5.23.: TTR-diagram at 600°C with weld material and varying applied stresses

Figure 5.24 compares the simulated TTR-curve at 625°C with the experimental creep rupture data for P91 weld material from Böhler. The only variations regarding input data compared to figure 5.22 are the new service temperature and the variation of the prefactor a_1 from 22 to 17.

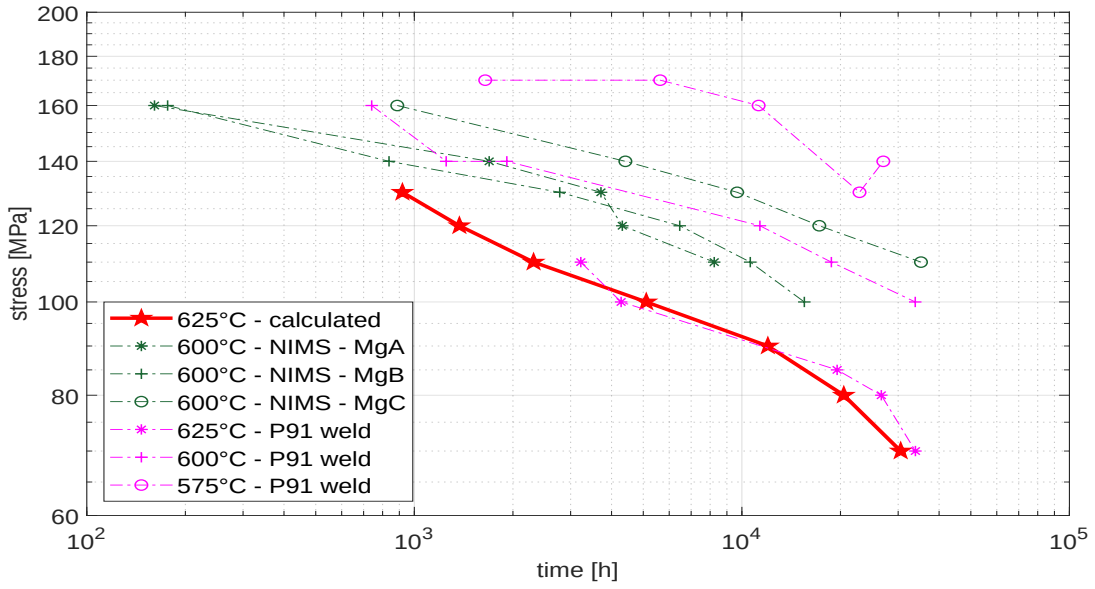

Figure 5.24.: TTR-diagram at 625°C with weld material and varying applied stresses

Figure 5.25 compares the simulated TTR-curve at 575°C with the experimental creep rupture data for P91 weld material from Böhler. The only variations regarding input data compared to figure 5.22 are the new service temperature and the variation of the prefactor a_1 from 22 to 25.

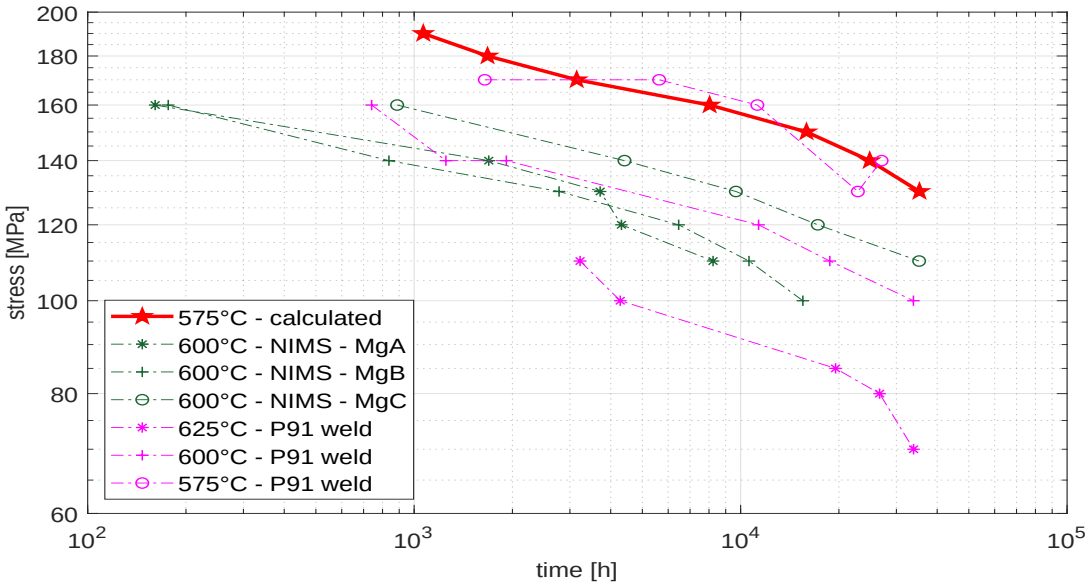

Figure 5.25.: TTR-diagram at 575°C with weld material and varying applied stresses

6. Evaluation and discussion

In this and the following chapter, the results found will be put into a meaningful context and evaluated with the insights gained during the work on this thesis.

6.1. EBSD data

The determined subgrain sizes in the range of about 1 µm diameter by manual counting of grain boundaries via mean interception method shall be given more trust than the automatically calculated subgrain diameter of 4.09 µm. Upon taking a closer look on the grainmap figure, there are a lot of disconnected borders, which may have mislead the algorithm (see figure 5.2 on page 33).

The comparison of these values with the reported sizes of subgrains and prior austenitic grains by Riedlsperger [12] is very interresting. The reported size for P91 base metal is:

- 76 µm for the PAGS and 0.56 µm for the subgrain size.

For the fine grain heat-affected zone:

- 9 µm for the PAGS and 0.51 µm for the subgrain size.

The prior austenitic grain size estimated from figure 5.4 lies in range of 50 to 75 µm.

So the microstructure found in the weld material is very similar to already known P91 base material [12]. This is in line with the comparable creep strengths of the weld material and the NIMS base metals (see e.g. figure 5.23 on page 46).

The influence of the post weld heat treatment cannot be accessed retrospectively, because no weld sample without PWHT is available but the findings would be interesting for sure.

6.2. MatCalc results

The creation of the Stepped Equilibrium and and Scheil-Gulliver diagrams were quite straightforward, problems with the code regarding custom composition sets were already mentioned in chapter 4.

The Scheil-Gulliver overview-diagram (figure 5.8 on page 37) shows very nicely that titanium nitrides precipitate and solidify in the melt before any iron phases are formed. Depending on the chemical composition, a peritectic phase transformation takes also place, as can be seen in the diagram.

Regarding the precipitation kinetic simulation, when looking at the mean diameter diagram (figure 5.17) the coarsening of the vanadium nitrides on the austenitic grain boundaries might have had a very huge impact on the subsequent creep simulation. As it turns out, the relatively low values in the number density diagram (5.18) and the phase fraction diagram (figure 5.16) certify that this phase will have no significant numerical impact.

Although the implementation of the modified Z-phase in the script may be described improvable as mentioned, the growth of the precipitates as well as the increase in phase fraction scales very nicely over the course of all temperature ranges.

Usually the formation of the modified Z-phase is discussed as a damage mechanism (chapter 2.3). Nevertheless, in the current implementation of the creep model this phase counts as an ordinary precipitate, since the impact of the corresponding dissolution of VN is already considered physically within the effective glide velocity of mobile dislocations.

6.3. The current state of MatCalc databases

All results obtained from the MatCalc simulations have to be seen under one special premise: The professional, up-to-date MatCalc ME databases are unfortunately not openly available for scientific purposes and I got no access to them during the writing of this thesis. In contrast to the freely accessible databases, they offer some enhancements in the descriptions of boride precipitates. [70]

In addition to that, the 2017 ME_Fe1.1 release changelog claims to have following notable improvements that would surely affect P91: [72]

- Improved phase stabilities in stainless steel of Laves phase and ferrite phase)
- Improvement of thermodynamic Fe-Nb base for simulations of microalloyed steel
- Corrected carbide stabilities in Fe-Cr-Mn-C (M_7C_3 was too stable)
- Reproduction of stabilisation of Cr_2N by Vanadium

ME_Fe1.2 major updates: [72]

- Reassessment of Sigma-phase stability and composition
- Reassessment of austenite/ferrite relative phase fractions in high-alloyed stainless steels

On a final note, all these changes clearly affect the simulations for P91, but without the chance to test the databases, it is not possible to quantify the amount of improvement the use of these databases would bring to the simulations or in which way the results would deviate.

6.4. Discussion of the governing equations

In the equation system two dissimilar variables for climb velocities are present: v_c is calculated by equation 3.17 and later used in Eq. 3.7 to calculate the effective glide velocity v_{eff}.

In contrast, v_{cc} is set at a constant velocity and is part of e.g. equation 3.8 to calculate the evolution of the mobile dislocation density.

This distinction between v_c and v_{cc} lead to better performance of the model because v_c is applicable when interactions between dislocations and precipitates are handled. The constant v_{cc} with an value of $9.70 \cdot 10^{-14}$ m/s is applicable on dislocation-dislocation-interactions. [1]

The origin of the multiplicative pre-factor a_1 of the glide velocity (Eq. 3.6 on page 17) is quite simple: Any unknown effects of temperature, stress and microstructure present on the dislocation glide velocity are corrected by it. The variable Ω_{mult} with an value of 21.8 was introduced during the transition to the new backstress-concept and implementation of v_{eff}. It serves (at least for the moment) as a correcting factor for the amount of atomic volumes that are being displaced during dislocation movement. At least in theory, these variables may be replaced by an enhanced mechanistic equation system at some point in the future.

As a first step, the correct ratio of a_1 and Ω_{mult} should be found with respect to temperature, stress and material condition. In this case, the glide velocity would be correct for more than just one temperature.

As it is implemented for now, the model has to be calibrated with plentiful experimental data in order to ascertain the pre-factor a_1 with sufficient precision. If this task is not carried out properly, the model is expected to result in over- or under-predictions of the final service lifetime.

6.5. MatLab creep model results

To get a good fit to the reference creep curves at 650°C (figure 5.19 on page 44) to compare the results of the new SRKSF-model to the SRKS-model from Schmid [1], some input data had to be modified: All model parameters for the start microstructures are listed in tables 4.3 and 4.4 in chapter 4.1 on page 24.

The start dislocation densities noted in these tables are about one third of the values used by Schmid [1] or reported in the literature, e.g. by El-Azim [73].

This, in combination with the variation of the prefactor a_1, resulted in much better fits of the creeps curves and TTR-diagrams. This is justifiable, because the experimental determination of dislocation densities is not trivial and the values from literature show also wide variations. [74]

The 'S'-type shape which was very apparent the TTR-curve from Schmid was not completely eliminated with the new model, but was straightened by a significant amount (see figure 5.20 on page 44). The reason for this deviation (which is not found in experiments) is currently still unclear.

Finally, the same procedure for the reference NIMS creep curve at 600°C also shows an acceptable fit (figure 5.21 on page 45).

Initially fitted only in one point, the extrapolation with higher and lower stresses (figure 5.22 on page 45) at otherwise identical parameters show only minimal deviations from the experimental data.

The simulated weld material at 600°C fits also very nicely to the experimental data, only one small adjustment of a_1 was needed to get an excellent fit (figure 5.23 on page 46)

Still calibrated for 600°C with again small adjustments to a_1, the TTR-curves for weld material at 625°C (fig. 5.24 on page 46) and 575°C (fig. 5.25 on page 47) show only minimal deviation from the experimental data.

As can be seen in figure 5.23 on page 46, the experimentally determined creep resistance of the weld material lies exactly between the TTR-curves from NIMS [9].

As a conclusion, it seems very unlikely that the weld material will be the weakest point during service time. This role will most likely be fulfilled by the nearby fine grain heat-affected zone. This assumption is backed by the microstructural configuration seen in the EBSD-pictures.

A final assessment on the performance of the model as a whole will take place in the next chapter.

7. Conclusion

During the work on this thesis, many milestones could be reached.

7.1. Evaluation of the supporting framework

The new Stepped Equilibrium and Scheil-Gulliver scripts proved to be valuable tools for an easier understanding of all phase stabilities and compositions as well as enabling a convenient calculation of the material's matrix composition.

The rewritten and extended Precipitation Kinetics script now bundles all thermal treatments in ONE unified script. Calculations for base metal, fine grain heat-affected zones and weld material will be of use for subsequent works in this field. It also includes a first working implementation of modified Z-phase precipitation and transformation.

The comprehensive and time-intensive rework of the Matlab code has already paid off many times. The comfortable automatic TTR-curve creation via automatic loops saves a lot of time and hassle.

The improved GUI with added access to many different datasets at once and also the possibility to combine them in any combination also simplifies and speeds up the daily work with the model, especially when more than one person is working on it at once.

7.2. Performance of the model

By combined efforts of the IMAT-modelling group under B. Sonderegger, the new backstress concept and the creation of a formulation for the implementation of the effective glide velocity v_{eff} (Eq. 3.7 on page 17) was realised and tested successfully.

The current hybrid model SRKSF now shows to predict primary, secondary and tertiary creep stages fairly well. Still, a low number of fit parameters are nonetheless necessary for the phenomenological part of the model. These parameters represent real physical quantities and could be determined separately of creep experiments, at least in principle.

Nevertheless, the model is capable to directly compare the TTR-curves of different material conditions relative to each other with sufficing precision.

It must be borne in mind that a purely physical model can never be assumed complete, but only appropriate and precise enough until a superior model is available. This means the newer model is either 'more accurate', 'possesses the same accuracy, but needs less fit parameters' or is 'suited for a wider range of cases'.

8. Outlook

Regarding the model, at least some parameters have to be investigated further: The multiplicative pre-factor a_1 on the glide velocity of dislocations in combination with the dislocation movement displacement factor Ω_{mult} as well as the parameter A, which is quantifying the cavitation damage. These parameters currently depend on stress, temperature and microstructure and have to be fitted to experimentally determined creep curves. Finding a physical basis for these variables (or basically any other fit-parameters) would enhance the predictability of the model in the future. The final goal would be a model with values for stress, temperature and starting microstructure as the only input parameters.

At this moment it is still not clear how generally (for which materials) the model can be applied. More methodical tests of one single material (e.g. P91) at different stresses, temperatures and start-microstructures are required. Once the results and the model have been validated, further testing and cross-checking with other materials may be started systematically.

The performance of Matlab regarding the calculation time could be improved further, one idea is to pre-calculate all interpolations of the MatCalc- precipitation kinetics simulation for all timesteps needed. The interpolation of this data via the 'interp1 function' is responsible for about 80% of the total calculation time in Matlab. The microstructural data does not change between the Matlab loops for calculating different stresses with one dataset, so the interpolated data from the first run could be saved and reused.

Maybe there are still some new effective ways to shorten the very long calculation times of MatCalc. With every phase and element used, the calculation time grows exponentially and unfortunately MatCalc is bound to a single calculation thread. Hopefully, future versions will utilize the capabilities of modern multicore CPUs. One full simulation takes 6-18 hours, but adding only two or three components will extent the time to days or even weeks. If one manages to maintain the accuracy of the simulation while using fewer elements, phases or other settings, the speedup would be tremendous. As a starting point, a more reliable implementation of the modified Z-phase precipitation would be a major improvement.

Many of these challenges will be tackled during the FWF-Project P 31374 (2018-2022) funded by the Austrian Science Fund. As one part of the whole project, B. Sonderegger, F. Riedlsperger and G. Zuderstorfer will transfer the creep model to the programming language C++. This will massively improve the handling and utilisation of microstructural data while offering a substantial speedup in calculations. It will also enable the creation of a more versatile and potent GUI as well as offer the potential of modular management of all formulas and dependencies.

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Appendix A.

Scripts MatCalc

Equi-scheil-fast-BF-final.mcs 1

```
$$ + + + + + PREAMBLE + + + + +

Author: Bernhard Fercher
date: 2018-11-30

Thermodynamic database: mc_fe_v2.059.tdb released 2016-07-26
Diffusion database: mc_fe_v2.011.ddb released 2016-10-19
Physical database: 1.03 released 2009-06-19
This is a script for MatCalc version 6.01 (rel 1.003) released 2018-04-26

This is a MatCalc-Script mainly used to aquire chemical data with the help of equilibrium and Scheil-Gulliver calculations
in P91 steel for following precipitation kinetics calculations. Adapt for P92 or FB2.

elements used: Fe - Al Co Cr Cu Nb Ni Mn Mo Si Ti V W - B C N P S

phases tested: LIQUID FCC_A1 BCC_A2 M23C6 M6C M7C3 LAVES_PHASE SIGMA ALN ALN_EQU BN_HP4 M2B FE24C10 CU2S ZET
Custom composition sets created: NbC VN TiN

+ + + + +  END OF PREAMBLE + + + + + $$

set-variable-string variable=version string=Equi-scheil-fast-BF-final

$ + + + + + PREPARE WORKSPACE + + + + +

use-module module-name=core
close-workspace options=f
new-workspace

set-log-file tracing=enable $ creates a log file in the userdirectory / logdirectory

$ + + + + + Check for MatCalc Version + + + + +

if (matcalc_version<6011003)
send-dialog-string string="MatCalc version must be 6.01 (rel 1.003) or higher. Stopping script."
stop-run-script
endif

$ + + + + + LOAD ELEMENTS AND PHASES + + + + +

open-thermodynamic-database file-name=mc_fe_v2.059.tdb

select-elements elements=Fe Va Si Mn Cr Ni Mo V Nb W Cu Ti Al Co P B N S C
select-phases phases=LIQUID FCC_A1 BCC_A2 M23C6 LAVES_PHASE SIGMA ALN BN_HP4 M2B CU2S ZET ALN_EQU $ HCP_A3 M6C M7C3 FE24C10

read-thermodynamic-database

read-physical-database file-name=physical_data.pdb $ loaded for diagrams later. MatCalc 6.01 crashes if this file is loaded after the calculations

$ create custom compositon sets

$ ATTENTION: too much elements in MX-sets create calculation (iteration) -errors, check in log-files


change-phase-status FCC_A1#01 set-flag=suspended

create-new-phase parent-phase=FCC_A1 composition-set constituents=:Cr,Fe,Mo,Mn,Ni,W,Nb%:C%,N,B,VA: phase-name=NbC
$change-phase-status phase-name=NbC set-flag=enforce-major-constituents
create-new-phase parent-phase=FCC_A1 composition-set constituents=:Cr,Fe,Mo,Mn,Ni,W,V%:N%,C,B,VA: phase-name=VN
$change-phase-status phase-name=VN set-flag=enforce-major-constituents
create-new-phase parent-phase=FCC_A1 composition-set constituents=:Cr,Fe,Mo,Mn,Ni,W,Ti%:N%,C,B,VA: phase-name=TiN
```

Figure A.1.: MatCalc-script: Stepped Equilibrium and Scheil-Gulliver (p.1)

```
61  $change-phase-status phase-name=TiN set-flag=enforce-major-constituents
62
63  $ + + + + + SPECIMEN SELECTION + + + + +
64  $ Could be rewritten for direct filename-input in console if really needed, for now
    (few specimens) this solution is better
65
66  $ P91_weld_Hxx (P91 weld material) (enter different values for Matrix composition if
    you want to)
67  set-variable-string variable=specimen string=13A40739001P
68  set-variable-string variable=material string=2CF4B10T-Y2046C04
69  set-variable-string variable=info1 string=5310_C9MV-Ti-FD_H23_1,2
70  set-variable-string variable=info2 string=P91_Hxx_regular
71  set-reference-element element=FE
72  enter-composition type=weight-percent composition=C=0.110 Si=0.21 Mn=0.79 Cr=8.83
    Ni=0.51 Mo=0.98 V=0.21 Nb=0.049 Cu=0.02 W=0.05 N=0.049 S=0.0039 B=0.001 Al=0.007
    Ti=0.033 P=0.013 Co=0.05
73
74   $ + + + + + STEPPED EQUILIBRIUM CALCULATION + + + + +
75
76  set-temperature-celsius temperature=1000
77  set-automatic-startvalues
78  calculate-equilibrium
79
80  rename-current-buffer new-buffer-name=equilibrium
81
82  set-step-option type=temperature
83  set-step-option range start=400 stop=1600 scale=C step-width=5
84  step-equilibrium
85
86  $ + + + + + CREATE AND MODIFY MAIN DIAGRAM + + + + +
87
88  new-gui-window type-id=p1
89  set-variable-value wid_equi active_frame_id $ save windows id to variable
90  set-gui-window-property window-id=wid_equi buffer-name=equilibrium $ attach to
    buffer window
91
92  move-gui-window displace window-id=. x-origin=0 y-origin=0 width=500 height=850
93  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes
94  set-gui-window-property window-id=. default-x-axis-data=T$C
95  set-gui-window-property window-id=. default-x-axis-title=temperature [°C]
96  set-plot-option plot-id=. series new buffer F$*
97  set-plot-option plot-id=. y-axis-title=phase fraction
98
99  $ a lot of html-commands are working in MatCalc for formatting
100 set-plot-option plot-id=. plot-title=<div align="left"> <small> MatCalc equilibrium
    calculation for<table> <tr> <td><i>specimen: </i> "#specimen"</td> <td> <i>
    material: </i> "#material"</th>  </tr> <tr>  <td>"#info1"</td>  <td> "#info2"</td>
    </tr> </small></div>
101
102 set-plot-option plot-id=. y-axis-type=log
103 set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes
104 set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes
105 set-plot-option plot-id=. grid which-grid=minor enable-x-axis=yes
106 set-plot-option plot-id=. grid which-grid=minor enable-y-axis=yes
107 set-plot-option plot-id=. legend legend-alignment=right
108 set-plot-option plot-id=. legend style=none
109 set-plot-option plot-id=. y-axis-scaling=1..0.00001
110 set-line-thickness plot-frame-id=2 line-thickness=3
111
112
113 $ + + + + + REMOVE PHASES IN PLOT AND LEGEND + + + + +
114 $ if calculating a new material activate all phases
115 set-plot-option plot-id=. series remove series-index=-1 series-name=F$FCC_A1#01
116 $set-plot-option plot-id=. series remove series-index=-1 series-name=F$LAVES_PHASE
117 set-plot-option plot-id=. series remove series-index=-1 series-name=F$LAVES_PHASE#01
118 set-plot-option plot-id=. series remove series-index=-1 series-name=F$LAVES_PHASE#02
119 set-plot-option plot-id=. series remove series-index=-1 series-name=F$ALN
120 $ set-plot-option plot-id=. series remove series-index=-1 series-name=F$M6C
121 $ set-plot-option plot-id=. series remove series-index=-1 series-name=F$M7C3
```

Figure A.2.: MatCalc-script: Stepped Equilibrium and Scheil-Gulliver (p.2)

```
122  $ set-plot-option plot-id=. series remove series-index=-1 series-name=F$FE24C10
123
124  $set-plot-option plot-id=. series rename series-index=-1 series-name=F$LAVES_PHASE
     new-name=F$LAVES_PH $Template for renaming phases
125
126  $ + + + + + EXPORT DIAGRAMS to PDFs + + + + +
127  $ Switch to export directory, export with specimen name, and change back
128  $format-variable-string variable=equilibrium_name format-string="%s%s-%s-%s" export/
     #info2 equi #specimen
129  $format-variable-string variable=equilibrium_name format-string="%s%s-%s" export/
     #info2 equi
130  $export-plot-to-file plot-id=#id format=pdf file-name=#equilibrium_name
131  $set-variable-value variable=id value=id+1
132
133  $ stop-run-script
134
135  $ + + + + + Scheil-Gulliver + + + + +
136
137  create-calc-buffer new-buffer-name=scheil
138  select-calc-buffer buffer-name=scheil
139
140  set-automatic-startvalues
141  set-temperature-celsius temperature=1525
142  calculate-equilibrium
143
144  set-step-option type=scheil
145  set-step-option range start=1525 stop=1000 step-width=1
146  set-step-option scheil-dependent-phase=liquid
147
148
149  $ IMPORTANT: Try other values below if the Scheil-calculation gives errors for new
     materials, often appearing at the peritectic range
150  $(first calculation to circumvent some odd behaviour of MatCalc)
151
152  set-step-option scheil-minimum-liquid-fraction=0.30 $ VARY THIS VALUE IF THE SCHEIL
     CALCULATION GIVES ERRORS
153
154  set-step-option scheil-create-phases-automatically=yes
155  set-step-option scheil-back-diffusion element=C yes
156  set-step-option scheil-back-diffusion element=B yes
157  set-step-option scheil-back-diffusion element=S yes
158  set-step-option scheil-back-diffusion element=P yes
159  set-step-option scheil-back-diffusion element=N yes
160
161  step-equilibrium  $perform first quick scheil calculation to create new solid phases
     (otherwise you would have to create all additional phases manually)
162
163  $ Define Scheil parameters for the final calculation
164  set-step-option scheil-minimum-liquid-fraction=0.01
165
166  $ Define peritectic transformation phases
167  create-new-phase parent-phase=fcc_a1 transformation-equilibrium
168  create-new-phase parent-phase=fcc_a1 transformation-solid
169
170  $ Define peritectic transformation
171  create-global-transformation new-transformation-name=peritectic
172  set-transformation-option transformation-name=peritectic type=full-equilibrium
173  set-transformation-option transformation-name=peritectic from-phase=bcc_a2_s
174  set-transformation-option transformation-name=peritectic to-phase=fcc_a1_s
175  set-transformation-option transformation-name=peritectic equilib-phase=fcc_a1_t
176  set-transformation-option transformation-name=peritectic temperature-range
     upper-temperature-threshold=1600 lower-temperature-threshold=1000
     temperature-in-C=yes
177  set-transformation-option transformation-name=peritectic active=yes
178
179  step-equilibrium $Perform final Scheil-Gulliver calculation.
180
181  $calculate the combined phases for the diagrams: Bulk composition + last solidified
     layer
```

Figure A.3.: MatCalc-script: Stepped Equilibrium and Scheil-Gulliver (p.3)

```
182  set-function-expression function=F$BCC_A2_COM expression=F$BCC_A2_S+F$BCC_A2
183  set-function-expression function=F$FCC_A1_COM expression=F$FCC_A1_S+F$FCC_A1
184  set-function-expression function=F$FCC_TR_COM expression=F$FCC_A1_T+F$FCC_A1_TS
185  set-function-expression function=F$TIN_COM expression=F$TIN_S+F$TIN
186
187
188  $ + + + + + CREATE AND MODIFY MAIN DIAGRAM + + + + +
189
190  new-gui-window type-id=p1
191  set-variable-value wid_scheil active_frame_id $ save windows id to variable
192  set-gui-window-property window-id=wid_scheil buffer-name=scheil $ attach to buffer
     window
193
194  move-gui-window displace window-id=. x-origin=0 y-origin=0 width=500 height=850
195  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes
196  set-gui-window-property window-id=. default-x-axis-data=T$C
197  set-gui-window-property window-id=. default-x-axis-title=temperature [°C]
198
199  $ Manually check which phases exist within the temperature range of the calculation
     and add them
200  set-plot-option plot-id=. series new buffer
     F$LIQUID
201  set-plot-option plot-id=. series new buffer F$BCC_A2_COM
202  set-plot-option plot-id=. series new buffer F$FCC_A1_COM
203  set-plot-option plot-id=. series new buffer F$FCC_TR_COM
204  set-plot-option plot-id=. series new buffer F$TIN_COM
205  set-plot-option plot-id=. y-axis-title=phase fraction
206
207  load-buffer-state line-index=-1
208  format-variable-string variable=temp_string format-string="%d°C" T$C
209
210
211  $ Hint: a lot of HTML-commands work in MatCalc for formatting
212  set-plot-option plot-id=. plot-title=<div align="left"> <small> MatCalc
     Scheil-Gulliver calculation down to 1% residual melt at #temp_string <table> <tr>
     <td><i>specimen: </i> #specimen </td> <td> <i> material: </i> "#material"</th>
     </tr> <tr>  <td> #info1 </td>  <td> #info2 </td>  </tr> </small></div>
213
214  set-plot-option plot-id=. y-axis-type=log
215  set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes
216  set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes
217  set-plot-option plot-id=. grid which-grid=minor enable-x-axis=yes
218  set-plot-option plot-id=. grid which-grid=minor enable-y-axis=yes
219  set-plot-option plot-id=. legend legend-alignment=right
220  set-plot-option plot-id=. legend style=none
221  set-plot-option plot-id=. y-axis-scaling=1..0.00001
222  set-line-thickness plot-frame-id=3 line-thickness=3
223
224
225  $ + + + + + EXPORT DIAGRAMS to PDFs + + + + +
226
227  $format-variable-string variable=scheil_name format-string="%s%s-%s" export/ #info2
     scheil_log
228  $export-plot-to-file plot-id=#id format=pdf file-name=#scheil_name
229  $set-variable-value variable=id value=id+1
230
231
232  $ + + + + + SAVE PROJECT + + + + +
233
234  format-variable-string variable=workspacename format-string="%s_%s" #version #info2
235
236  save-workspace #workspacename
237
```

Figure A.4.: MatCalc-script: Stepped Equilibrium and Scheil-Gulliver (p.4)

Precip-BF-final.mcs 1

```
1  $$ + + + + + PREAMBLE + + + + +
2
3  Author: Bernhard Fercher
4  date: 2018-11-30
5
6  Script for simulation of precipitation kinetics of multi-stage heat treatment and
   HT-service of 9% Cr-steel (Grade 91)
7  Script is inspired and uses parts of the MatCalc steel template script and work of
   F. Riedlsperger (2017) IMAT TU Graz.
8
9  Thermodynamic database: mc_fe_v2.059.tdb released 2016-07-26
10 Diffusion database: mc_fe_v2.011.ddb released 2016-10-19
11 Physical database: 1.03 released 2009-06-19
12 This is a script for MatCalc version 6.01 (rel 1.003) released 2018-04-26
13
14 Hint: Crosscheck your calculated results on different PCs when possible, sometimes
   MatCalc may yield different results depending on CPU, operating system or other
   things not yet determined.
15 Tested for identical results on: Intel i7-4930k, 32 GB Ram, Windows 7 Prof. 64 bit
   and i5-8250U, 8GB RAM, Windows 10 Prof. 64 bit
16
17 + + + + +  END OF PREAMBLE + + + + + $$
18
19 set-variable-string variable=version string=Precip-BF-Final $ set string for savefile
20
21 $ + + + + + PREPARE WORKSPACE + + + + +
22
23 use-module module-name=core
24 close-workspace options=f
25 new-workspace
26
27 set-log-file tracing=enable $ creates a log file in the userdirectory / logdirectory
28
29 $ Check for MatCalc Version
30 if (matcalc_version<6011003)
31 send-dialog-string string="MatCalc version must be 6.01 (rel 1.003) or higher.
   Stopping script."
32 stop-run-script
33 endif
34
35 move-gui-window show console $ show console window for selections later
36
37 send-console-string string="."
38 send-console-string string="1: Calculate BM (base metal, no welding, no PWHT)"
39 send-console-string string="2: Calculate FGHAZ (fine grain heat-affected zone)"
40 send-console-string string="3: Calculate WELD (Pure Weld Material, no FGHAZ, no BM)"
41 input-variable-value variable=userselection input-string="Select which Material to
   calculate"
42
43 send-console-string string="."
44 input-variable-value variable=T_serv input-string="Type in service (creep)
   temperature [°C]"
45
46 $ stop-run-script $ debugging line
47
48 $ + + + + + GLOBAL VARIABLES + + + + +
49
50 set-variable-string variable=scale_range string=1e10..1e23 $ unified scaling for
   histogram windows
51
52 $ The number of required precipitation classes possible depends on the performance
   of the CPU. Especially when using low values,
53 $ results may differ but give a much faster calculation. Higher heating or cooling
   rates need higher values to get accurate results.
54 $ After adjusting heating and cooling rates, the number of size classes used has to
   be checked thoroughly.
55 $ Default is 25- lower value worsens accuracy dramatically, 50 minimum for is
   strongly recommended, especially for the z phase
56
```

Figure A.5.: MatCalc-script: Precipitation kinetics (p.1)

```
57  set-variable-value variable=npc value=50 $ set number prec. classes
58  set-variable-value variable=npc_laves value=50 $ prec. classes for laves phase
59  set-variable-value variable=npc_m23c6 value=50 $ prec. classes for M23C6
60  set-variable-value variable=npc_aln value=50 $ prec. classes for AlN
61  set-variable-value variable=npc_vn value=50 $ prec. classes for VN(mart,s) +
    VN(aust,g)
62  set-variable-value variable=npc_nbc value=50 $ prec. classes for NbC(mart,d) +
    NbC(mart,s)
63  set-variable-value variable=npc_Z value=50 $ prec. classes for Z
64
65
66  set-variable-value variable=mdef value=1 $ matrix diff. enhancement factor during
    PWHT and service is 1 (8 for faster diffusion in FGHAZ)
67  set-variable-value variable=mdef_sgb value=1 $ matrix diff. enhancement at subgrain
    boundaries
68
69
70  set-variable-value variable=eie_zet value=0.590 $ equivalent interf. energy for
    Z-phase nucleation
71  set-variable-value variable=nucl_const_zet value=1e-12 $ nucleation constant for
    matrix-Z-phase
72  set-variable-value variable=zmnr value=5e-10 $ minimum nucleation radius
73
74
75  set-variable-value variable=lav_ict value=1452 $ interface correction temperature
    [K] for laves (Molybdän) Fe2Mo, Value calculated by F. Riedelsperger
76  $ set-variable-value lav_ict 1452 $ interface correction temperature [K] for laves
    (Wolfram) Fe2W has to be calculated, expected to be about 1840K
77
78  $ The equilibrium solution temperature of laves phase is close to the service
    temperature of 600C.
79  $ Therefore the interface between the matrix and laves phase becomes diffuse instead
    of sharp. To
80  $ handle this state, an interface correction temperature of 1452K for is applied.
81  $ A higher interface correction temp. like 1600K causes coarsening of laves phase.
82  $ A good estimation for the range of Laves interface correction temperature can be
    made by creating a
83  $ binary system of Fe-Mo or Fe-W (depending on the chemical composition of Grade 91)
    and finding the maximum
84  $ dissolution temperature for Laves phase when varying Fe- and Mo-content [wt-%],
    which in this case gave 1477 K.
85  $ Further optimization of this value led to 1452 K, which now can be used at any
    temperature level of service.
86  $ 600 degrees of service temperature in theory demand the same interface correction
    temperature as 650 degrees
87
88
89  set-variable-value variable=dda value=1e11 $ dislocation density in austenite
90
91
92  set-variable-value variable=ddm value=1.5e14       $ dislocation density in
    martensite after 0h service
93  set-variable-value variable=ddm_100h value=1.48e14 $ calculation of ddm reduction
    according to extrapolation formula from S. Yadav:
94  set-variable-value variable=ddm_200h value=1.47e14 $ ddm=2.39257*10^16*t^(-0.57315),
    where ddm= dislocation density and t= time.
95  set-variable-value variable=ddm_300h value=1.46e14 $ IMPORTANT: primary creep has to
    be neglected to receive good results
96  set-variable-value variable=ddm_400h value=1.45e14 $ Consequently, a start value of
    1,5e14 m^(-2) for dislocation density is defined
97  set-variable-value variable=ddm_500h value=1.44e14 $ values from F. Riedelsperger
98  set-variable-value variable=ddm_600h value=1.43e14
99  set-variable-value variable=ddm_700h value=1.42e14
100 set-variable-value variable=ddm_800h value=1.41e14
101 set-variable-value variable=ddm_900h value=1.4e14
102 set-variable-value variable=ddm_1000h value=1.39e14
103 set-variable-value variable=ddm_1250h value=1.36e14
104 set-variable-value variable=ddm_1500h value=1.34e14
105 set-variable-value variable=ddm_2000h value=1.3e14
```

Figure A.6.: MatCalc-script: Precipitation kinetics (p.2)

```
106  set-variable-value variable=ddm_2500h value=1.26e14
107  set-variable-value variable=ddm_3000h value=1.22e14
108  set-variable-value variable=ddm_3500h value=1.19e14
109  set-variable-value variable=ddm_4000h value=1.15e14
110  set-variable-value variable=ddm_4500h value=1.13e14
111  set-variable-value variable=ddm_5000h value=1.1e14
112  set-variable-value variable=ddm_6000h value=1.05e14
113  set-variable-value variable=ddm_9000h value=9.31e13
114  set-variable-value variable=ddm_12000h value=8.44e13
115  set-variable-value variable=ddm_15000h value=7.76e13
116  set-variable-value variable=ddm_20000h value=6.9e13
117  set-variable-value variable=ddm_25000h value=6.26e13
118  set-variable-value variable=ddm_30000h value=5.76e13
119  set-variable-value variable=ddm_40000h value=5.02e13
120  set-variable-value variable=ddm_50000h value=4.5e13
121  set-variable-value variable=ddm_60000h value=4.1e13
122  set-variable-value variable=ddm_70000h value=3.78e13
123  set-variable-value variable=ddm_80000h value=3.53e13
124  set-variable-value variable=ddm_90000h value=3.31e13
125  set-variable-value variable=ddm_100000h value=3.13e13
126
127
128  set-variable-value variable=T_ms value=400 $ martensite start temperature // check
     for value for your specifc material
129  $ (326 bis 599)
130
131  set-variable-value variable=T_weld_fghaz value=950 $ virtual welding peak
     temperature in FGHAZ (higher than T_aust)
132
133  set-variable-value variable=T_trans value=833 $ martensite to austenite
     transformation temperature reaustenitization
134  $ check for value for your spezific material
135
136  $ The austenitic grain size (ags) was determined through analysis of EBSD data with
     OIM software, with
137  $ respect to dislocation angles between 18 and 50 degrees.
138  $ To account for prior austenitic grain boundaries (that were not clearly visible),
     a correction factor
139  $ based on the Mackenzie distribution was introduced with which the PAGS values
     derived from linear
140  $ intercept method (manual procedure) were corrected.
141
142
143  set-variable-value variable=ags value=76e-6 $ austenitic grain size in BM [=76µm]
144  set-variable-value variable=sgs value=0.56e-6 $ subgrain size in BM [=0,56µm]
145  $ set-variable-value variable=sgef value=5 $ subgrain elongation factor BM [BUG in
     6.01, don't use]
146
147  set-variable-value variable=agsfghaz value=9e-6 $ austenitic grain size of FGHAZ
     [=9µm]
148  set-variable-value variable=sgsfghaz value=1.45e-6 $ subgrain size in FGHAZ [=1,45µm]
149  $ set-variable-value variable=sgeffghaz value=1 $ subgrain elongation factor in
     FGHAZ [=1] [BUG in 6.01, don't use]
150
151  set-variable-value variable=agsweld value=8.04e-6 $ austenitic grain size of weld
     [=8,04µm]
152  set-variable-value variable=sgsweld value=4.09e-6 $ subgrain size in weld [=4,09µm]
153
154  $ variables for heat treatments
155  set-variable-value variable=T_aust value=1050 $ normalizing temperature (values from
     921 to x)
156  set-variable-value variable=time_aust value=2*60*60 $ normalizing time (=2h)
157
158  set-variable-value variable=T_temp value=770 $ tempering temperature (values from
     551 to x)
159  set-variable-value variable=time_temp value=2*60*60 $ tempering time (=2h)
160
161  set-variable-value variable=T_pwht value=760 $ PWHT temperature (values from 651 to x)
162  set-variable-value variable=time_pwht value=4*60*60 $ PWHT time (=4h)
```

Figure A.7.: MatCalc-script: Precipitation kinetics (p.3)

```
163
164  $ precipitate shape
165  set-variable-value variable=sf_m7c3 value=3     $ shape factor for m7c3 precipitates
166  set-variable-value variable=sf_cem value=3      $ shape factor for cementite
     precipitates
167
168
169  $ + + + + + DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES + + + + +
170
171  open-thermodynamic-database file-name=mc_fe_v2.059.tdb $ open thermodynamic database
172
173  select-elements elements=Fe Va Si Mn Cr Ni Mo V Nb W Al N C $ Cu Ti Co B S P select
     elements, change composition accordingly
174  select-phases phases=liquid fcc_a1 bcc_a2 laves_phase m23c6 hcp_a3 aln zet m7c3
     cementite $ hcp_a3 select phases
175  read-thermodynamic-database $ read thermodynamic database
176
177  set-variable-string variable=samplename string=P91_Hxx $add samplename for diagram
     and workspace naming
178
179  $ P91 Hxx composition from SCHEIL-Calculation. Insert composition of 99% Matrix
     (Original analysis minus content of 1% residual melt) Calculation via excel-table
180  enter-composition type=weight-percent composition=C=0.105 Si=0.208 Mn=0.774 Cr=8.769
     Ni=0.506 Mo=0.957 V=0.204 Nb=0.0278 N=0.0477 W=0.0492 Al=0.00706
181  $ Ti=0.0332 S=0.00225 P=0.0127 B=0.000591 Co=0.0495 Cu=0.0199
182
183  read-mobility-database file-name=mc_fe_v2.011.ddb $ read diffusion data
184
185  $ + + + + + CHANGE PHASE STATUS ETC.
186
187  create-new-phase parent-phase=FCC_A1 composition-set constituents=:Cr,Fe,Nb%:C%,VA:
     phase-name=NbC
188  $ change-phase-status phase-name=NbC set-flag=enforce-major-constituents
189  create-new-phase parent-phase=FCC_A1 composition-set constituents=:Cr,Fe,V%:N%,VA:
     phase-name=VN
190  $ change-phase-status phase-name=VN set-flag=enforce-major-constituents
191  $ create-new-phase parent-phase=FCC_A1 composition-set
     constituents=:Cr,Fe,Ti%:N%,VA: phase-name=TiN
192  $ change-phase-status phase-name=TiN set-flag=enforce-major-constituents
193
194
195
196  change-phase-status phase-name=FCC_A1#01 set-flag=suspended $ suspend fcc_a1#01, it
     is replaced by simple phases NbC, TiN and VN
197
198
199  $ suspend hcp_a3 and kids, is replaced by simple phases
200
201  create-new-phase parent-phase=hcp_a3 composition-set constituents=:CR%,NB,V:N%,C,VA:
     phase-name=Cr2N $ Cr2-nitride
202  $ create-new-phase parent-phase=hcp_a3 composition-set constituents=:MO%,NB,V:C%,VA:
     phase-name=Mo2C $ Mo2C
203  change-phase-status phase-name=hcp_a3 set-flag=suspended
204  change-phase-status phase-name=hcp_a3#01 set-flag=suspended
205  change-phase-status phase-name=hcp_a3#02 set-flag=suspended
206  change-phase-status phase-name=hcp_a3#03 set-flag=suspended
207
208  change-phase-status phase-name=laves_phase#01 set-flag=suspended
209  $ change-phase-status phase-name=laves_phase#02 set-flag=suspended
210
211
212  $$ + + + + + DEBUG-Lines to check for Errors + + + + +
213
214  set-temperature-celsius temperature=1000
215  set-automatic-startvalues
216  calculate-equilibrium
217  rename-current-buffer new-buffer-name=equilibrium
218  set-step-option type=temperature
219  set-step-option range start=400 stop=1600 scale=C step-width=5
```

Figure A.8.: MatCalc-script: Precipitation kinetics (p.4)

```
220  step-equilibrium
221  $$
222
223  $ stop-run-script
224
225
226  $ + + + + + HEAT TREATMENTS + + + + +
227
228  if (userselection==1)
229
230  $ PART I: HARDENING
231
232  create-tm-treatment tm-treatment-name=hardening $ create heat treatment part I:
233
234  append-tmt-segment tm-treatment-name=hardening $ casting process (START)
235  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=austenite $ define precipitation domain
236  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-start-temperature=1500 $ define start temperature
237  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_ms temperature-gradient=0.1 $ end temperature and cooling
     rate
238  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from solution treatment to martensite start $ comment
239
240  append-tmt-segment tm-treatment-name=hardening $ casting process- change to
     martensite (END)
241  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=martensite $ define precipitation domain
242  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=25 temperature-gradient=0.1 $ Tend + cooling rate
243  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from martensite start to room temperature $ comment
244
245  append-tmt-segment tm-treatment-name=hardening $ heating to normalize (START)
246  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=40 temperature-gradient=0.0083 $ Tend + heating rate
247  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from room temperature 40 degrees $ comment
248
249  append-tmt-segment tm-treatment-name=hardening $ heating to normalize
250  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_trans temperature-gradient=0.0444 $ T_trans (Tend) +
     heating rate
251  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from 40 degrees to A3 temperature $ comment
252
253  append-tmt-segment tm-treatment-name=hardening $ heating to normalize- change to
     austenite
254  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=austenite $ define precipitation domain
255  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=920 temperature-gradient=0.0444 $ Tend + heating rate
256  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from A3 temperature to 920 degrees $ comment
257
258  append-tmt-segment tm-treatment-name=hardening $ heating to normalize
259  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_aust temperature-gradient=0.0181 $ Tend + heating rate
260  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from 920 degrees to austenitization temperature $ comment
261
262  append-tmt-segment tm-treatment-name=hardening $ normalizing (HOLDING)
263  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=time_aust $ Tdot + delta_t
264  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=isothermal holding for 2 h at austenitization temperature $ comment
265
266  append-tmt-segment tm-treatment-name=hardening $ cooling process
```

Figure A.9.: MatCalc-script: Precipitation kinetics (p.5)

```
267  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=800 temperature-gradient=0.0694 $ Point T4 Tend + cooling rate
268  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from austenitization temperature to 800 degrees $ comment
269
270  append-tmt-segment tm-treatment-name=hardening $ cooling process
271  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=600 temperature-gradient=0.0556 $ Point T5 Tend + cooling rate
272  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 800 degrees to 600 degrees $ comment
273
274  append-tmt-segment tm-treatment-name=hardening $ cooling process
275  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=460 temperature-gradient=0.0389 $ Point T6 Tend + cooling rate
276  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 600 degrees to 460 degrees $ comment
277
278  append-tmt-segment tm-treatment-name=hardening $ cooling process
279  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_ms temperature-gradient=0.0278 $ T_ms (=Tend)+ cooling rate
280  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=quenching to martensite start temperature $ comment
281
282  append-tmt-segment tm-treatment-name=hardening $ cooling process- change to
     martensite
283  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=martensite $ define precipitation domain
284  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=360 temperature-gradient=0.0278 $ Tend + Point T7 (=Tend) +
     cooling rate
285  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from martensite start temperature to 360 degrees $ comment
286
287  append-tmt-segment tm-treatment-name=hardening $ cooling process
288  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=320 temperature-gradient=0.0111 $ Point T8 (=Tend) + cooling
     rate
289  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 360 degrees to 320 degrees $ comment
290
291  append-tmt-segment tm-treatment-name=hardening $ cooling process
292  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=260 temperature-gradient=0.0167 $ Point T9 (=Tend) + cooling
     rate
293  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 320 to 260 degrees
294
295  append-tmt-segment tm-treatment-name=hardening $ cooling process (END)
296  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=25 temperature-gradient=0.013 $ T10 (=room temperature) +
     cooling rate (extrapolated)
297  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 260 degrees to room temperature
298
299  $ END OF PART I: HARDENING
300
301  $ PART II: TEMPERING
302
303  create-tm-treatment tm-treatment-name=tempering $ second heat treatment
304
305  append-tmt-segment tm-treatment-name=tempering $ heating to temper (START)
306  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     segment-start-temperature=25 $ define start temperature
307  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     precipitation-domain=martensite $ define precipitation domain
308  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=80 temperature-gradient=0.0306 $ Point T2 (=Tend) + heating
     rate
309  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
```

Figure A.10.: MatCalc-script: Precipitation kinetics (p.6)

```
      segment-comment=heating from room temperature to 80 degrees $ comment
310
311   append-tmt-segment tm-treatment-name=tempering $ heating to temper
312   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_temp temperature-gradient=0.0295 $ T_temp (=Tend) +
      heating rate
313   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=heating from 80 degrees to tempering temperature $ comment
314
315   append-tmt-segment tm-treatment-name=tempering $ tempering (HOLDING)
316   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_dot+delta_t
      temperature-gradient=0 segment-delta-time=time_temp $ Tdot + delta_t
317   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=annealing for 2 h $ comment
318
319   append-tmt-segment tm-treatment-name=tempering $ cooling process
320   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=550 temperature-gradient=0.0244 $ Point T3 (=Tend) + cooling
      rate
321   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from tempering temperature to 550 degrees $ comment
322
323   append-tmt-segment tm-treatment-name=tempering $ cooling process
324   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=420 temperature-gradient=0.0181 $ Point T4 (=Tend) + cooling
      rate
325   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from 550 degrees to 420 degrees $ comment
326
327   append-tmt-segment tm-treatment-name=tempering $ cooling process
328   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=360 temperature-gradient=0.0111 $ Tend + cooling rate
329   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from 420 degrees to 360 degrees $ comment
330
331   append-tmt-segment tm-treatment-name=tempering $ cooling process
332   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=250 temperature-gradient=0.0134 $ Point T5 (=Tend) + cooling
      rate
333   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from 360 degrees to 250 degrees $ comment
334
335   append-tmt-segment tm-treatment-name=tempering $ append segment 2
336   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=25 temperature-gradient=0.01 $ Point T6 (=Tend) + cooling
      rate (extrapolated)
337   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling to room temperature $ comment
338
339   $ END OF PART II: TEMPERING
340
341   elseif (userselection==2)
342
343
344   $ PART I: HARDENING
345
346   create-tm-treatment tm-treatment-name=hardening $ create heat treatment part I:
347
348   append-tmt-segment tm-treatment-name=hardening $ casting process (START)
349   edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
      precipitation-domain=austenite $ define precipitation domain
350   edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
      segment-start-temperature=1500 $ define start temperature
351   edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_ms temperature-gradient=0.1 $ end temperature and cooling
      rate
352   edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
      segment-comment=cooling from solution treatment to martensite start $ comment
353
```

Figure A.11.: MatCalc-script: Precipitation kinetics (p.7)

```
354  append-tmt-segment tm-treatment-name=hardening $ casting process- change to
     martensite (END)
355  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=martensite $ define precipitation domain
356  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=25 temperature-gradient=0.1 $ Tend + cooling rate
357  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from martensite start to room temperature $ comment
358
359  append-tmt-segment tm-treatment-name=hardening $ heating to normalize (START)
360  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=40 temperature-gradient=0.0083 $ Tend + heating rate
361  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from room temperature 40 degrees $ comment
362
363  append-tmt-segment tm-treatment-name=hardening $ heating to normalize
364  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_trans temperature-gradient=0.0444 $ T_trans (Tend) +
     heating rate
365  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from 40 degrees to A3 temperature $ comment
366
367  append-tmt-segment tm-treatment-name=hardening $ heating to normalize- change to
     austenite
368  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=austenite $ define precipitation domain
369  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=920 temperature-gradient=0.0444 $ Tend + heating rate
370  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from A3 temperature to 920 degrees $ comment
371
372  append-tmt-segment tm-treatment-name=hardening $ heating to normalize
373  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_aust temperature-gradient=0.0181 $ Tend + heating rate
374  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=heating from 920 degrees to austenitization temperature $ comment
375
376  append-tmt-segment tm-treatment-name=hardening $ normalizing (HOLDING)
377  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=time_aust $ Tdot + delta_t
378  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=isothermal holding for 2 h at austenitization temperature $ comment
379
380  append-tmt-segment tm-treatment-name=hardening $ cooling process
381  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=800 temperature-gradient=0.0694 $ Point T4 Tend + cooling rate
382  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from austenitization temperature to 800 degrees $ comment
383
384  append-tmt-segment tm-treatment-name=hardening $ cooling process
385  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=600 temperature-gradient=0.0556 $ Point T5 Tend + cooling rate
386  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 800 degrees to 600 degrees $ comment
387
388  append-tmt-segment tm-treatment-name=hardening $ cooling process
389  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=460 temperature-gradient=0.0389 $ Point T6 Tend + cooling rate
390  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 600 degrees to 460 degrees $ comment
391
392  append-tmt-segment tm-treatment-name=hardening $ cooling process
393  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_ms temperature-gradient=0.0278 $ T_ms (=Tend)+ cooling rate
394  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=quenching to martensite start temperature $ comment
395
396  append-tmt-segment tm-treatment-name=hardening $ cooling process- change to
     martensite
```

Figure A.12.: MatCalc-script: Precipitation kinetics (p.8)

```
397  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     precipitation-domain=martensite $ define precipitation domain
398  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=360 temperature-gradient=0.0278 $ Tend + Point T7 (=Tend) +
     cooling rate
399  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from martensite start temperature to 360 degrees $ comment
400
401  append-tmt-segment tm-treatment-name=hardening $ cooling process
402  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=320 temperature-gradient=0.0111 $ Point T8 (=Tend) + cooling
     rate
403  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 360 degrees to 320 degrees $ comment
404
405  append-tmt-segment tm-treatment-name=hardening $ cooling process
406  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=260 temperature-gradient=0.0167 $ Point T9 (=Tend) + cooling
     rate
407  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 320 to 260 degrees
408
409  append-tmt-segment tm-treatment-name=hardening $ cooling process (END)
410  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=25 temperature-gradient=0.013 $ T10 (=room temperature) +
     cooling rate (extrapolated)
411  edit-tmt-segment tm-treatment-name=hardening tm-treatment-segment=.
     segment-comment=cooling from 260 degrees to room temperature
412
413  $ END OF PART I: HARDENING
414
415  $ PART II: TEMPERING
416
417  create-tm-treatment tm-treatment-name=tempering $ second heat treatment
418
419  append-tmt-segment tm-treatment-name=tempering $ heating to temper (START)
420  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     segment-start-temperature=25 $ define start temperature
421  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     precipitation-domain=martensite $ define precipitation domain
422  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=80 temperature-gradient=0.0306 $ Point T2 (=Tend) + heating
     rate
423  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     segment-comment=heating from room temperature to 80 degrees $ comment
424
425  append-tmt-segment tm-treatment-name=tempering $ heating to temper
426  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=T_temp temperature-gradient=0.0295 $ T_temp (=Tend) +
     heating rate
427  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     segment-comment=heating from 80 degrees to tempering temperature $ comment
428
429  append-tmt-segment tm-treatment-name=tempering $ tempering (HOLDING)
430  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=time_temp $ Tdot + delta_t
431  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     segment-comment=annealing for 2 h $ comment
432
433  append-tmt-segment tm-treatment-name=tempering $ cooling process
434  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=550 temperature-gradient=0.0244 $ Point T3 (=Tend) + cooling
     rate
435  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
     segment-comment=cooling from tempering temperature to 550 degrees $ comment
436
437  append-tmt-segment tm-treatment-name=tempering $ cooling process
438  edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
     segment-end-temperature=420 temperature-gradient=0.0181 $ Point T4 (=Tend) + cooling
```

Figure A.13.: MatCalc-script: Precipitation kinetics (p.9)

```
      rate
439   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from 550 degrees to 420 degrees $ comment
440
441   append-tmt-segment tm-treatment-name=tempering $ cooling process
442   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=360 temperature-gradient=0.0111 $ Tend + cooling rate
443   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from 420 degrees to 360 degrees $ comment
444
445   append-tmt-segment tm-treatment-name=tempering $ cooling process
446   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=250 temperature-gradient=0.0134 $ Point T5 (=Tend) + cooling
      rate
447   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling from 360 degrees to 250 degrees $ comment
448
449   append-tmt-segment tm-treatment-name=tempering $ append segment 2
450   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=25 temperature-gradient=0.01 $ Point T6 (=Tend) + cooling
      rate (extrapolated)
451   edit-tmt-segment tm-treatment-name=tempering tm-treatment-segment=.
      segment-comment=cooling to room temperature $ comment
452
453   $ END OF PART II: TEMPERING
454
455   $ PART III: WELDING
456
457   create-tm-treatment tm-treatment-name=welding $ third heat treatment
458
459   append-tmt-segment tm-treatment-name=welding $ heating to welding peak (START)
460   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-start-temperature=25 $ define start temperature for HT
461   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      precipitation-domain=martensite $ define precipitation domain
462   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_trans temperature-gradient=37.848 $ T_trans (=Tend) +
      heating rate (37,848 °C/s)
463   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=heating from room temperature to A3 temperature $ comment
464
465   append-tmt-segment tm-treatment-name=welding $ heating to welding peak- change to
      austenite
466   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      precipitation-domain=austenite $ define precipitation domain
467   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_weld_fghaz temperature-gradient=37.848 $ T_weld_fghaz
      (=950°C) + heating rate (37,848 °C/s)
468   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=heating from A3 to welding peak temperature $ comment
469
470   append-tmt-segment tm-treatment-name=welding $ welding peak (HOLDING)
471   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_dot+delta_t
      temperature-gradient=0 segment-delta-time=5 $ Tdot + delta_t
472   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter austenite
      initial-grain-diameter=agsfghaz $ modification of austenitic grain size in FGHAZ
473   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=exposed to welding peak temperature for 5 s
474
475   append-tmt-segment tm-treatment-name=welding $ cooling process
476   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=600 temperature-gradient=11.25 $ Point T2 (=Tend) + cooling
      rate
477   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling from peak weld temperature to 600 degrees $ comment
478
479   append-tmt-segment tm-treatment-name=welding $ cooling process
480   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
```

Figure A.14.: MatCalc-script: Precipitation kinetics (p.10)

```
      segment-end-temperature=T_ms temperature-gradient=6.188 $ T_ms (=Tend) + cooling rate
481   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter martensite
      initial-grain-diameter=agsfghaz $ modification of martensite grain size in FGHAZ
482   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter martensite
      initial-subgrain-diameter=sgsfghaz $ modification of martensite lath size in FGHAZ
483   $ edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter martensite
      subgrain-elongation-factor=sgeffghaz $ modification of martensite lath elongation
      factor in FGHAZ
484   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=quenching from 600 degrees to martensite start temperature $ comment
485
486   append-tmt-segment tm-treatment-name=welding $ cooling process- change to martensite
487   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      precipitation-domain=martensite $ define precipitation domain
488   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=325 temperature-gradient=6.188 $ Point T3 (=Tend) + cooling
      rate
489   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling form martensite start temperature to 325 degrees $ comment
490
491   append-tmt-segment tm-treatment-name=welding $ cooling process
492   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=109 temperature-gradient=1.836 $ Point T4 (=Tend) + cooling
      rate
493   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling from 325 degrees to 109 degrees
494
495   append-tmt-segment tm-treatment-name=welding $ cooling process (END)
496   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=25 temperature-gradient=1 $ Tend + cooling rate (extrapolated)
497   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling to room temperature $ comment
498
499   $ END OF PART III: WELDING
500
501   $ PART IV: PWHT
502
503   create-tm-treatment tm-treatment-name=pwht $ fourth heat treatment
504
505   append-tmt-segment tm-treatment-name=pwht $ append segment 0 "tempering"
506   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-start-temperature=25 $ define start temperature for HT
507   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      precipitation-domain=martensite $ define precipitation domain
508   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_pwht temperature-gradient=0.022 $ Tend + heating
      rate(=80C/h)
509   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=Heating to PWHT temperature with 80C/h $ comment
510
511   append-tmt-segment tm-treatment-name=pwht $ append segment 1
512   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_dot+delta_t
      temperature-gradient=0 segment-delta-time=time_pwht $ Tdot + delta_t
513   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=annealing for 120min $ comment
514
515   append-tmt-segment tm-treatment-name=pwht $ append segment 2
516   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=650 temperature-gradient=0.022 $ Tend + cooling rate(=80C/h)
517   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=cooling to 650C $ comment
518
519   append-tmt-segment tm-treatment-name=pwht $ append segment 3
520   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=560 temperature-gradient=0.022 $ Tend + cooling rate(=80C/h)
521   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
```

Figure A.15.: MatCalc-script: Precipitation kinetics (p.11)

```
      segment-comment=cooling to 560C $ comment
522
523   append-tmt-segment tm-treatment-name=pwht $ append segment 4
524   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=510 temperature-gradient=0.014 $ Tend + cooling rate(=50C/h)
525   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=cooling to 510C $ comment
526
527   append-tmt-segment tm-treatment-name=pwht $ append segment 5
528   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=470 temperature-gradient=0.011 $ Tend + cooling rate(=40C/h)
529   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=cooling to 470C $ comment
530
531   append-tmt-segment tm-treatment-name=pwht $ append segment 6
532   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=25 temperature-gradient=0.008 $ Tend + cooling rate(=30C/h)
533   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=cooling to room temperature $ comment
534
535   $  END OF PART IV: PWHT
536
537   elseif (userselection==3)
538
539   $ PART I: WELDING
540
541   create-tm-treatment tm-treatment-name=welding $ create welding:
542
543   append-tmt-segment tm-treatment-name=welding $ casting process (START)
544   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-start-temperature=1500 $ define start temperature
545   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      precipitation-domain=austenite $ define precipitation domain
546   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=800 temperature-gradient=35 $ Point T2 (=Tend) + cooling rate
547   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling from peak weld temperature to 800 degrees $ comment
548
549   append-tmt-segment tm-treatment-name=welding $ cooling process
550   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=500 temperature-gradient=15 $ Point T4 (=Tend) + cooling
      rate t8/5 20 seconds
551   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling from 800 degrees to 500 degrees
552
553   append-tmt-segment tm-treatment-name=welding $ cooling process
554   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_ms temperature-gradient=7 $ T_ms (=Tend) + cooling rate
555   $ edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter martensite
      subgrain-elongation-factor=sgeffghaz $ modification of martensite lath elongation
      factor in FGHAZ
556   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling from 500 degrees to martensite start temperature $ comment
557
558   append-tmt-segment tm-treatment-name=welding $ cooling process- change to martensite
559   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      precipitation-domain=martensite $ define precipitation domain
560   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=325 temperature-gradient=4 $ Point T3 (=Tend) + cooling rate
561   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling form martensite start temperature to 260 degrees $
      Zwischenlagentemp
562
563   append-tmt-segment tm-treatment-name=welding $ cooling process (END)
564   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=25 temperature-gradient=1 $ Tend + cooling rate (extrapolated)
565   edit-tmt-segment tm-treatment-name=welding tm-treatment-segment=.
      segment-comment=cooling to room temperature $ comment
```

Figure A.16.: MatCalc-script: Precipitation kinetics (p.12)

```
566
567   $ END OF PART I: WELDING
568
569
570   $ PART II: PWHT
571
572   create-tm-treatment tm-treatment-name=pwht $ second heat treatment
573
574   append-tmt-segment tm-treatment-name=pwht $ append segment 0 "tempering"
575   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-start-temperature=25 $ define start temperature for HT
576   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      precipitation-domain=martensite $ define precipitation domain
577   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_pwht temperature-gradient=80/3600 $ Tend + heating
      rate(=80C/h)
578   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=Heating to PWHT temperature with 80C/h $ comment
579
580   append-tmt-segment tm-treatment-name=pwht $ append segment 1
581   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_dot+delta_t
      temperature-gradient=0 segment-delta-time=time_pwht $ Tdot + delta_t
582   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=annealing for time_pwht min $ comment
583
584   append-tmt-segment tm-treatment-name=pwht $ append segment 6
585   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=25 temperature-gradient=80/3600 $ Tend + cooling rate(=80C/h)
586   edit-tmt-segment tm-treatment-name=pwht tm-treatment-segment=.
      segment-comment=cooling to room temperature $ comment
587
588   $  END OF PART II: PWHT
589
590   else
591
592   endif
593
594   $ PART V: SERVICE
595
596   create-tm-treatment tm-treatment-name=service $ fifth heat treatment
597
598   append-tmt-segment tm-treatment-name=service $ append segment 1 "tempering"
599   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      segment-start-temperature=25 $ define start temperature
600   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      precipitation-domain=martensite $ define precipitation domain
601   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_end+T_dot
      segment-end-temperature=T_serv temperature-gradient=0.033 $ Tend + heating rate
602   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      segment-comment=Heating to service temperature $ comment
603
604   append-tmt-segment tm-treatment-name=service $ append segment 2
605   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
      temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
606   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter martensite
      equilibrium-dislocation-density=ddm_100h
607   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      segment-comment=isothermal service $ comment: sum=100h
608
609   append-tmt-segment tm-treatment-name=service $ append segment 3
610   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
      temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
611   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      post-segment-command=set-precipitation-parameter martensite
      equilibrium-dislocation-density=ddm_200h
612   edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
      segment-comment=isothermal service $ comment: sum=200h
613
```

Figure A.17.: MatCalc-script: Precipitation kinetics (p.13)

```
614  append-tmt-segment tm-treatment-name=service $ append segment 4
615  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
616  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_300h
617  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=300h
618
619  append-tmt-segment tm-treatment-name=service $ append segment 5
620  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
621  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_400h
622  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=400h
623
624  append-tmt-segment tm-treatment-name=service $ append segment 6
625  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
626  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_500h
627  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=500h
628
629  append-tmt-segment tm-treatment-name=service $ append segment 7
630  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
631  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_600h
632  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=600h
633
634  append-tmt-segment tm-treatment-name=service $ append segment 8
635  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
636  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_700h
637  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=700h
638
639  append-tmt-segment tm-treatment-name=service $ append segment 9
640  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
641  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_800h
642  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=800h
643
644  append-tmt-segment tm-treatment-name=service $ append segment 10
645  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
646  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_900h
647  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=900h
648
649  append-tmt-segment tm-treatment-name=service $ append segment 11
650  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=100*60*60 $ Tdot + delta_t
651  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_1000h
```

Figure A.18.: MatCalc-script: Precipitation kinetics (p.14)

```
652  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=1000h
653
654  append-tmt-segment tm-treatment-name=service $ append segment 12
655  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=250*60*60 $ Tdot + delta_t
656  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_1250h
657  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=1250h
658
659  append-tmt-segment tm-treatment-name=service $ append segment 13
660  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=250*60*60 $ Tdot + delta_t
661  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_1500h
662  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=1500h
663
664  append-tmt-segment tm-treatment-name=service $ append segment 14
665  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
666  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_2000h
667  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=2000h
668
669  append-tmt-segment tm-treatment-name=service $ append segment 15
670  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
671  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_2500h
672  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=2500h
673
674  append-tmt-segment tm-treatment-name=service $ append segment 16
675  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
676  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_3000h
677  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=3000h
678
679  append-tmt-segment tm-treatment-name=service $ append segment 17
680  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
681  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_3500h
682  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=3500h
683
684  append-tmt-segment tm-treatment-name=service $ append segment 18
685  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
686  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_4000h
687  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=4000h
688
689  append-tmt-segment tm-treatment-name=service $ append segment 19
690  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
```

Figure A.19.: MatCalc-script: Precipitation kinetics (p.15)

```
691  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_4500h
692  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=4500h
693
694  append-tmt-segment tm-treatment-name=service $ append segment 20
695  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=500*60*60 $ Tdot + delta_t
696  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_5000h
697  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=5000h
698
699  append-tmt-segment tm-treatment-name=service $ append segment 21
700  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=1000*60*60 $ Tdot + delta_t
701  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_6000h
702  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=6000h
703
704  append-tmt-segment tm-treatment-name=service $ append segment 22
705  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=3000*60*60 $ Tdot + delta_t
706  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_9000h
707  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=9000h
708
709  append-tmt-segment tm-treatment-name=service $ append segment 23
710  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=3000*60*60 $ Tdot + delta_t
711  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_12000h
712  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=12000h
713
714  append-tmt-segment tm-treatment-name=service $ append segment 24
715  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=3000*60*60 $ Tdot + delta_t
716  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_15000h
717  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=15000h
718
719  append-tmt-segment tm-treatment-name=service $ append segment 25
720  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=5000*60*60 $ Tdot + delta_t
721  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_20000h
722  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=20000h
723
724  append-tmt-segment tm-treatment-name=service $ append segment 26
725  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=5000*60*60 $ Tdot + delta_t
726  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_25000h
727  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=25000h
728
```

Figure A.20.: MatCalc-script: Precipitation kinetics (p.16)

```
729  append-tmt-segment tm-treatment-name=service $ append segment 27
730  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=5000*60*60 $ Tdot + delta_t
731  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_30000h
732  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=30000h
733
734  append-tmt-segment tm-treatment-name=service $ append segment 28
735  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
736  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_40000h
737  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=40000h
738
739  append-tmt-segment tm-treatment-name=service $ append segment 29
740  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
741  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_50000h
742  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=50000h
743
744  append-tmt-segment tm-treatment-name=service $ append segment 30
745  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
746  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_60000h
747  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=60000h
748
749  append-tmt-segment tm-treatment-name=service $ append segment 31
750  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
751  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_70000h
752  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=70000h
753
754  append-tmt-segment tm-treatment-name=service $ append segment 32
755  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
756  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_80000h
757  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=80000h
758
759  append-tmt-segment tm-treatment-name=service $ append segment 33
760  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
761  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_90000h
762  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=90000h
763
764  append-tmt-segment tm-treatment-name=service $ append segment 34
765  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=. T_dot+delta_t
     temperature-gradient=0 segment-delta-time=10000*60*60 $ Tdot + delta_t
766  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     post-segment-command=set-precipitation-parameter martensite
     equilibrium-dislocation-density=ddm_100000h
```

Figure A.21.: MatCalc-script: Precipitation kinetics (p.17)

```
767  edit-tmt-segment tm-treatment-name=service tm-treatment-segment=.
     segment-comment=isothermal service $ comment: sum=100000h
768
769  $stop-run-script
770
771  $ + + + + + PRECIPITATION DOMAINS, PRECIPITATES
772
773  if (userselection==3)
774
775  create-precipitation-domain new-domain-name=austenite $ austenite is precipitation
     domain = matrix
776  set-precipitation-parameter austenite general thermodynamic-matrix-phase=FCC_A1 $
     matrix phase of domain austenite
777  set-precipitation-parameter austenite equilibrium-dislocation-density=dda $
     dislocation density (=1e11 m^-2)
778  set-precipitation-parameter austenite initial-grain-diameter=agsweld $ austenite
     grain size
779
780  create-precipitation-domain new-domain-name=martensite  $ new matrix: martensite
781  set-precipitation-parameter martensite general thermodynamic-matrix-phase=BCC_A2 $
     define matrix structure
782  set-precipitation-parameter martensite equilibrium-dislocation-density=ddm $
     dislocation density (=1e14 m^-2)
783  set-precipitation-parameter martensite initial-grain-diameter=agsweld $ =austenite
     grain size WELD
784  set-precipitation-parameter martensite initial-subgrain-diameter=sgsweld $ subgrain
     size WELD
785  $ set-precipitation-parameter martensite subgrain-elongation-factor=sgef $ subgrain
     elongation factor [BUG in 6.01, don't use]
786
787  else
788
789  create-precipitation-domain new-domain-name=austenite $ austenite is precipitation
     domain = matrix
790  set-precipitation-parameter austenite general thermodynamic-matrix-phase=FCC_A1 $
     matrix phase of domain austenite
791  set-precipitation-parameter austenite equilibrium-dislocation-density=dda $
     dislocation density (=1e11 m^-2)
792  set-precipitation-parameter austenite initial-grain-diameter=ags $ austenite grain
     size
793
794  create-precipitation-domain new-domain-name=martensite  $ new matrix: martensite
795  set-precipitation-parameter martensite general thermodynamic-matrix-phase=BCC_A2 $
     define matrix structure
796  set-precipitation-parameter martensite equilibrium-dislocation-density=ddm $
     dislocation density (=1e14 m^-2)
797  set-precipitation-parameter martensite initial-grain-diameter=ags $ =austenite grain
     size
798  set-precipitation-parameter martensite initial-subgrain-diameter=sgs $ subgrain size
799  $ set-precipitation-parameter martensite subgrain-elongation-factor=sgef $ subgrain
     elongation factor [BUG in 6.01, don't use]
800
801  endif
802
803  $ PRECIPITATE PHASES
804
805  create-new-phase parent-phase=aln precipitate AlN(mart,di) $ new precipitate phase
     in martensite
806  set-precipitation-parameter aln_p0 number-of-size-classes=npc_aln $ use variable for
     prec. classes
807  set-precipitation-parameter aln_p0 nucleation-sites=dislocations $ nucleation sites
     are dislocations
808  set-precipitation-parameter aln_p0 use-volumetric-misfit-in-nucleation=yes
809  set-precipitation-parameter aln_p0 volumetric-misfit=0.27 $ use volumetric misfit
     value of 0.27
810  set-precipitation-parameter aln_p0
     restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
     precipitation domain
811  $ set-precipitation-parameter aln_p3 nucleate-only-with-valid-major-constituents=yes
```

Figure A.22.: MatCalc-script: Precipitation kinetics (p.18)

```
812
813   create-new-phase parent-phase=aln precipitate AlN(mart,sgb) $ new precipitate phase
      in martensite
814   set-precipitation-parameter aln_p1 number-of-size-classes=npc_aln $ use variable for
      prec. classes
815   set-precipitation-parameter aln_p1 nucleation-sites=subgrain-boundaries $ nucleation
      sites are dislocations
816   set-precipitation-parameter aln_p1 use-volumetric-misfit-in-nucleation=yes
817   set-precipitation-parameter aln_p1 volumetric-misfit=0.27 $ use volumetric misfit
      value of 0.27
818   set-precipitation-parameter aln_p1
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
819   $ set-precipitation-parameter aln_p5 nucleate-only-with-valid-major-constituents=yes
820
821   create-new-phase parent-phase=NBC precipitate NbC(aust,di) $ new precipitate phase
      in austenite
822   set-precipitation-parameter NBC_P0 number-of-size-classes=npc $ use variable for
      prec. classes
823   set-precipitation-parameter NBC_P0 nucleation-sites=dislocations $ nucleation sites
      are dislocations
824   set-precipitation-parameter NBC_P0
      restrict-nucleation-to-precipitation-domain=austenite  $ restrict nucleation to
      precipitation domain
825   set-precipitation-parameter NBC_P0 nucleate-only-with-valid-major-constituents=yes $
      nucleate only with valid major constituents
826   $ set-precipitation-parameter NbC_P0 use-volumetric-misfit-in-nucleation=yes
827   $ set-precipitation-parameter NbC_P0 volumetric-misfit=0.1
828   $ change-phase-status NBC_p0 set-flag=enforce-major-constituents
829
830   create-new-phase parent-phase=NBC precipitate NbC(aust,gb) $ new precipitate phase
      in austenite
831   set-precipitation-parameter NBC_P1 number-of-size-classes=npc $ use variable for
      prec. classes
832   set-precipitation-parameter NBC_P1 nucleation-sites=grain-boundaries $ nucleation
      sites are dislocations
833   set-precipitation-parameter NBC_P1
      restrict-nucleation-to-precipitation-domain=austenite  $ restrict nucleation to
      precipitation domain
834   set-precipitation-parameter NBC_P1 nucleate-only-with-valid-major-constituents=yes $
      nucleate only with valid major constituents
835
836   create-new-phase parent-phase=NBC precipitate NbC(aust,sgb) $ new precipitate phase
      in austenite
837   set-precipitation-parameter NBC_P2 number-of-size-classes=npc $ use variable for
      prec. classes
838   set-precipitation-parameter NBC_P2 nucleation-sites=subgrain-boundaries $ nucleation
      sites are dislocations
839   set-precipitation-parameter NBC_P2
      restrict-nucleation-to-precipitation-domain=austenite  $ restrict nucleation to
      precipitation domain
840   set-precipitation-parameter NBC_P2 nucleate-only-with-valid-major-constituents=yes $
      nucleate only with valid major constituents
841
842   create-new-phase parent-phase=nbc precipitate NbC(mart,di) $ new precipitate phase
      in martensite
843   set-precipitation-parameter nbc_p3 number-of-size-classes=npc_nbc $ use variable for
      prec. classes
844   set-precipitation-parameter nbc_p3 nucleation-sites=dislocations $ nucleation sites
      are dislocations
845   $ set-precipitation-parameter nbc_P1 use-volumetric-misfit-in-nucleation=yes
846   $ set-precipitation-parameter nbc_P1 volumetric-misfit=0.1
847   set-precipitation-parameter nbc_p3 nucleate-only-with-valid-major-constituents=yes $
      nucleate only with valid major constituents
848   set-precipitation-parameter nbc_p3
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
849   $ change-phase-status NBc_p1 set-flag=enforce-major-constituents
850
```

Figure A.23.: MatCalc-script: Precipitation kinetics (p.19)

```
851  create-new-phase parent-phase=nbc precipitate NbC(mart,gb) $ new precipitate phase
     in martensite
852  set-precipitation-parameter nbc_p4 number-of-size-classes=npc_nbc $ use variable for
     prec. classes
853  set-precipitation-parameter nbc_p4 nucleation-sites=grain-boundaries $ nucleation
     sites are dislocations
854  $ set-precipitation-parameter nbc_P1 use-volumetric-misfit-in-nucleation=yes
855  $ set-precipitation-parameter nbc_P1 volumetric-misfit=0.1
856  set-precipitation-parameter nbc_p4 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
857  set-precipitation-parameter nbc_p4
     restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
     precipitation domain
858  $ change-phase-status NBc_p1 set-flag=enforce-major-constituents
859
860  create-new-phase parent-phase=nbc precipitate NbC(mart,sgb) $ new precipitate phase
     in martensite
861  set-precipitation-parameter nbc_p5 number-of-size-classes=npc_nbc $ use variable for
     prec. classes
862  set-precipitation-parameter nbc_p5 nucleation-sites=subgrain-boundaries $ nucleation
     sites are dislocations
863  $ set-precipitation-parameter nbc_P1 use-volumetric-misfit-in-nucleation=yes
864  $ set-precipitation-parameter nbc_P1 volumetric-misfit=0.1
865  set-precipitation-parameter nbc_p5 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
866  set-precipitation-parameter nbc_p5
     restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
     precipitation domain
867  $ change-phase-status NBc_p1 set-flag=enforce-major-constituents
868
869  create-new-phase parent-phase=VN precipitate VN(aust,di) $ new precipitate phase VN
     in austenite
870  set-precipitation-parameter vn_p0 number-of-size-classes=npc_vn $ use variable npc
     for # of prec. classes
871  set-precipitation-parameter vn_p0 nucleation-sites=dislocations $ nucleation sites
     at grain boundaries
872  set-precipitation-parameter vn_p0 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
873  set-precipitation-parameter vn_p0
     restrict-nucleation-to-precipitation-domain=austenite $ restrict nucleation to
     precipitation domain
874  $ change-phase-status vn_p0 set-flag=enforce-major-constituents
875
876  create-new-phase parent-phase=VN precipitate VN(aust,gb) $ new precipitate phase VN
     in austenite
877  set-precipitation-parameter vn_p1 number-of-size-classes=npc_vn $ use variable npc
     for # of prec. classes
878  set-precipitation-parameter vn_p1 nucleation-sites=grain-boundaries $ nucleation
     sites at grain boundaries
879  set-precipitation-parameter vn_p1 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
880  set-precipitation-parameter vn_p1
     restrict-nucleation-to-precipitation-domain=austenite $ restrict nucleation to
     precipitation domain
881  $ change-phase-status vn_p0 set-flag=enforce-major-constituents
882
883  create-new-phase parent-phase=VN precipitate VN(aust,sgb) $ new precipitate phase VN
     in austenite
884  set-precipitation-parameter vn_p2 number-of-size-classes=npc_vn $ use variable npc
     for # of prec. classes
885  set-precipitation-parameter vn_p2 nucleation-sites=subgrain-boundaries $ nucleation
     sites at grain boundaries
886  set-precipitation-parameter vn_p2 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
887  set-precipitation-parameter vn_p2
     restrict-nucleation-to-precipitation-domain=austenite $ restrict nucleation to
     precipitation domain
888  $ change-phase-status vn_p0 set-flag=enforce-major-constituents
889
```

Figure A.24.: MatCalc-script: Precipitation kinetics (p.20)

```
890  create-new-phase parent-phase=VN precipitate VN(mart,di) $ new precipitate phase VN
     in martensite
891  set-precipitation-parameter vn_p3 number-of-size-classes=npc $ use variable npc for
     # of prec. classes
892  set-precipitation-parameter vn_p3 nucleation-sites=dislocations $ nucleation sites
     at dislocations
893  set-precipitation-parameter vn_p3 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
894  set-precipitation-parameter vn_p3
     restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
     precipitation domain
895  $ change-phase-status vn_p1 set-flag=enforce-major-constituents
896
897  create-new-phase parent-phase=VN precipitate VN(mart,gb) $ new precipitate phase VN
     in martensite
898  set-precipitation-parameter vn_p4 number-of-size-classes=npc $ use variable npc for
     # of prec. classes
899  set-precipitation-parameter vn_p4 nucleation-sites=grain-boundaries $ nucleation
     sites at dislocations
900  set-precipitation-parameter vn_p4 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
901  set-precipitation-parameter vn_p4
     restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
     precipitation domain
902  $ change-phase-status vn_p1 set-flag=enforce-major-constituents
903
904  create-new-phase parent-phase=VN precipitate VN(mart,sgb) $ new precipitate phase VN
     in martensite
905  set-precipitation-parameter vn_p5 number-of-size-classes=npc $ use variable npc for
     # of prec. classes
906  set-precipitation-parameter vn_p5 nucleation-sites=subgrain-boundaries $ nucleation
     sites at dislocations
907  set-precipitation-parameter vn_p5 nucleate-only-with-valid-major-constituents=yes $
     nucleate only with valid major constituents
908  set-precipitation-parameter vn_p5
     restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
     precipitation domain
909  $ change-phase-status vn_p1 set-flag=enforce-major-constituents
910
911  $ The M7C3 and Cementite precipitates are not stable at the creep temperature (600C)
     but they have to be
912  $ considered in the calculation due to the influence on the M23C6 evolution during
     heating and cooling treatments
913  $ which leads to a better agreement with experimental values of M23C6 diameter.
914
915  create-new-phase parent-phase=m7c3 precipitate alias-name=M7C3(mart,di)
916  set-precipitation-parameter m7c3_p0 number-of-size-classes=npc $ use variable for
     prec. classes
917  set-precipitation-parameter m7c3_p0 nucleation-sites=dislocations
918  set-precipitation-parameter m7c3_p0 shape-factor=sf_m7c3
919  set-precipitation-parameter m7c3_p0
     restrict-nucleation-to-precipitation-domain=martensite
920  set-precipitation-parameter m7c3_p0 nucleate-only-with-valid-major-constituents=yes
921
922  create-new-phase parent-phase=m7c3 precipitate alias-name=M7C3(mart,gb)
923  set-precipitation-parameter m7c3_p1 number-of-size-classes=npc $ use variable for
     prec. classes
924  set-precipitation-parameter m7c3_p1 nucleation-sites=grain-boundaries
925  set-precipitation-parameter m7c3_p1 shape-factor=sf_m7c3
926  set-precipitation-parameter m7c3_p1
     restrict-nucleation-to-precipitation-domain=martensite
927  set-precipitation-parameter m7c3_p1 nucleate-only-with-valid-major-constituents=yes
928
929  create-new-phase parent-phase=m7c3 precipitate alias-name=M7C3(mart,sgb)
930  set-precipitation-parameter m7c3_p2 number-of-size-classes=npc $ use variable for
     prec. classes
931  set-precipitation-parameter m7c3_p2 nucleation-sites=subgrain-boundaries
932  set-precipitation-parameter m7c3_p2 shape-factor=sf_m7c3
933  set-precipitation-parameter m7c3_p2
```

Figure A.25.: MatCalc-script: Precipitation kinetics (p.21)

```
      restrict-nucleation-to-precipitation-domain=martensite
934   set-precipitation-parameter m7c3_p2 nucleate-only-with-valid-major-constituents=yes
935
936   create-new-phase parent-phase=m23c6 precipitate alias-name=M23C6(mart,di)
937   set-precipitation-parameter m23c6_p0 number-of-size-classes=npc_m23c6 $ use variable
      for prec. classes
938   set-precipitation-parameter m23c6_p0 nucleation-sites=dislocations
939   set-precipitation-parameter m23c6_p0
      restrict-nucleation-to-precipitation-domain=martensite
940   set-precipitation-parameter m23c6_p0 nucleate-only-with-valid-major-constituents=yes
941
942   create-new-phase parent-phase=m23c6 precipitate alias-name=M23C6(mart,gb)
943   set-precipitation-parameter m23c6_p1 number-of-size-classes=npc_m23c6 $ use variable
      for prec. classes
944   set-precipitation-parameter m23c6_p1 nucleation-sites=grain-boundaries
945   set-precipitation-parameter m23c6_p1
      restrict-nucleation-to-precipitation-domain=martensite
946   set-precipitation-parameter m23c6_p1 nucleate-only-with-valid-major-constituents=yes
947
948   create-new-phase parent-phase=m23c6 precipitate alias-name=M23C6(mart,sgb)
949   set-precipitation-parameter m23c6_p2 number-of-size-classes=npc_m23c6 $ use variable
      for prec. classes
950   set-precipitation-parameter m23c6_p2 nucleation-sites=subgrain-boundaries
951   set-precipitation-parameter m23c6_p2
      restrict-nucleation-to-precipitation-domain=martensite
952   set-precipitation-parameter m23c6_p2 nucleate-only-with-valid-major-constituents=yes
953
954   create-new-phase parent-phase=cementite precipitate Cem(mart,di) $ new precipitate
      cementite in martensite
955   set-precipitation-parameter cementite_p0 number-of-size-classes=npc $ use variable
      for prec. classes
956   set-precipitation-parameter cementite_p0 nucleation-sites=dislocations $ nucleation
      sites at dislocations
957   set-precipitation-parameter cementite_p0 shape-factor=sf_cem
958   set-precipitation-parameter cementite_p0
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      prec. domain
959   set-precipitation-parameter cementite_p0
      nucleate-only-with-valid-major-constituents=yes
960
961   create-new-phase parent-phase=cementite precipitate Cem(mart,gb) $ new precipitate
      cementite in martensite
962   set-precipitation-parameter cementite_p1 number-of-size-classes=npc $ use variable
      for prec. classes
963   set-precipitation-parameter cementite_p1 nucleation-sites=grain-boundaries $
      nucleation sites at dislocations
964   set-precipitation-parameter cementite_p1 shape-factor=sf_cem
965   set-precipitation-parameter cementite_p1
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      prec. domain
966   set-precipitation-parameter cementite_p1
      nucleate-only-with-valid-major-constituents=yes
967
968   create-new-phase parent-phase=cementite precipitate Cem(mart,sgb) $ new precipitate
      cementite in martensite
969   set-precipitation-parameter cementite_p2 number-of-size-classes=npc $ use variable
      for prec. classes
970   set-precipitation-parameter cementite_p2 nucleation-sites=subgrain-boundaries $
      nucleation sites at dislocations
971   set-precipitation-parameter cementite_p2 shape-factor=sf_cem
972   set-precipitation-parameter cementite_p2
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      prec. domain
973   set-precipitation-parameter cementite_p2
      nucleate-only-with-valid-major-constituents=yes
974
975   create-new-phase parent-phase=laves_phase precipitate alias-name=Laves(mart,di)
976   set-precipitation-parameter laves_phase_p0 number-of-size-classes=npc_laves
977   set-precipitation-parameter laves_phase_p0 nucleation-sites=dislocations
```

Figure A.26.: MatCalc-script: Precipitation kinetics (p.22)

```
978  set-precipitation-parameter laves_phase_p0
     restrict-nucleation-to-precipitation-domain=martensite
979  set-precipitation-parameter laves_phase_p0
     nucleate-only-with-valid-major-constituents=yes
980  set-precipitation-parameter laves_phase_p0 diffuse-interface-energy-effect=yes $
     diffuse interface correction is set on
981  set-precipitation-parameter laves_phase_p0
     regular-solution-critical-temperature=lav_ict
982
983  create-new-phase parent-phase=laves_phase precipitate
     alias-name=Laves(mart,sgb)
984  set-precipitation-parameter laves_phase_p1 number-of-size-classes=npc_laves
985  set-precipitation-parameter laves_phase_p1 nucleation-sites=subgrain-boundaries
986  set-precipitation-parameter laves_phase_p1
     restrict-nucleation-to-precipitation-domain=martensite
987  set-precipitation-parameter laves_phase_p1
     nucleate-only-with-valid-major-constituents=yes
988  set-precipitation-parameter laves_phase_p1 diffuse-interface-energy-effect=yes $
     diffuse interface correction is set on
989  set-precipitation-parameter laves_phase_p1
     regular-solution-critical-temperature=lav_ict
990
991  create-new-phase parent-phase=Cr2N precipitate Cr2N(mart,di) $ new precipitate phase
     in martensite
992  set-precipitation-parameter Cr2N_p0 number-of-size-classes=npc $ use variable for
     prec. classes
993  set-precipitation-parameter Cr2N_p0 nucleation-sites=dislocations $ nucleation sites
     are dislocations
994  set-precipitation-parameter Cr2N_p0 nucleate-only-with-valid-major-constituents=yes
995  set-precipitation-parameter Cr2N_p0
     restrict-nucleation-to-precipitation-domain=martensite
996
997  create-new-phase parent-phase=Cr2N precipitate Cr2N(mart,gb) $ new precipitate phase
     in martensite
998  set-precipitation-parameter Cr2N_p1 number-of-size-classes=npc $ use variable for
     prec. classes
999  set-precipitation-parameter Cr2N_p1 nucleation-sites=grain-boundaries $ nucleation
     sites are dislocations
1000 set-precipitation-parameter Cr2N_p1 nucleate-only-with-valid-major-constituents=yes
1001 set-precipitation-parameter Cr2N_p1
     restrict-nucleation-to-precipitation-domain=martensite
1002
1003 create-new-phase parent-phase=Cr2N precipitate Cr2N(mart,sgb) $ new precipitate
     phase in martensite
1004 set-precipitation-parameter Cr2N_p2 number-of-size-classes=npc $ use variable for
     prec. classes
1005 set-precipitation-parameter Cr2N_p2 nucleation-sites=subgrain-boundaries $
     nucleation sites are dislocations
1006 set-precipitation-parameter Cr2N_p2 nucleate-only-with-valid-major-constituents=yes
1007 set-precipitation-parameter Cr2N_p2
     restrict-nucleation-to-precipitation-domain=martensite
1008
1009 $ Zet-phase has special settings due to the fact that it nucleates within the VN
     precipitates
1010 $ and nucleation is defined as special nucleation model for precipitation on
     particles with
1011 $ equivalent interfacial energy. Make sure that 'direct particle transformation' is
     selected as
1012 $ nucleation model. The value for the equivalent interfacial energy is basically
     unknown and must
1013 $ be considered as a fitting parameter. Presently, no physical model for Z-phase
     nucleation
1014 $ is available.
1015
1016 create-new-phase parent-phase=ZET precipitate Z(mart,vn_a_di) $ new prec. phase for
     Zet-phase in martensite
1017 set-precipitation-parameter zet_p0 number-of-size-classes=npc_z $ use variable for
     prec. classes
1018 set-precipitation-parameter zet_p0 nucleation-parent-precipitate=vn_p0 $ nucleation
```

Figure A.27.: MatCalc-script: Precipitation kinetics (p.23)

```
      sites are existing VN prec.
1019  set-precipitation-parameter zet_p0 equivalent-interface-energy=eie_zet $ use equiv.
      intf. energy
1020  set-precipitation-parameter zet_p0 nucleation-model=particle-related-transformation
      $ use direct particle transf. nucl. model
1021  set-precipitation-parameter zet_p0
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
1022  set-precipitation-parameter ZET_P0 minimum-nucleation-radius=zmnr
1023
1024  create-new-phase parent-phase=ZET precipitate Z(mart,vn_a_gb) $ new prec. phase for
      Zet-phase in martensite
1025  set-precipitation-parameter zet_p1 number-of-size-classes=npc_z $ use variable for
      prec. classes
1026  set-precipitation-parameter zet_p1 nucleation-parent-precipitate=vn_p1 $ nucleation
      sites are existing VN prec.
1027  set-precipitation-parameter zet_p1 equivalent-interface-energy=eie_zet $ use equiv.
      intf. energy
1028  set-precipitation-parameter zet_p1 nucleation-model=particle-related-transformation
      $ use direct particle transf. nucl. model
1029  set-precipitation-parameter zet_p1
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
1030  set-precipitation-parameter ZET_P1 minimum-nucleation-radius=zmnr
1031
1032  create-new-phase parent-phase=ZET precipitate Z(mart,vn_a_sgb) $ new prec. phase for
      Zet-phase in martensite
1033  set-precipitation-parameter zet_p2 number-of-size-classes=npc_z $ use variable for
      prec. classes
1034  set-precipitation-parameter zet_p2 nucleation-parent-precipitate=vn_p2 $ nucleation
      sites are existing VN prec.
1035  set-precipitation-parameter zet_p2 equivalent-interface-energy=eie_zet $ use equiv.
      intf. energy
1036  set-precipitation-parameter zet_p2 nucleation-model=particle-related-transformation
      $ use direct particle transf. nucl. model
1037  set-precipitation-parameter zet_p2
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
1038  set-precipitation-parameter ZET_P2 minimum-nucleation-radius=zmnr
1039
1040  create-new-phase parent-phase=ZET precipitate Z(mart,vn_m_di) $ new prec. phase for
      Zet-phase in martensite
1041  set-precipitation-parameter zet_p3 number-of-size-classes=npc_z $ use variable for
      prec. classes
1042  set-precipitation-parameter zet_p3 nucleation-parent-precipitate=vn_p3 $ nucleation
      sites are existing VN prec.
1043  set-precipitation-parameter zet_p3 equivalent-interface-energy=eie_zet $ use equiv.
      intf. energy
1044  set-precipitation-parameter zet_p3 nucleation-model=particle-related-transformation
      $ use direct particle transf. nucl. model
1045  set-precipitation-parameter ZET_P3
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
1046  set-precipitation-parameter ZET_P3 minimum-nucleation-radius=zmnr
1047
1048  create-new-phase parent-phase=ZET precipitate Z(mart,vn_m_gb) $ new prec. phase for
      Zet-phase in martensite
1049  set-precipitation-parameter zet_p4 number-of-size-classes=npc_z $ use variable for
      prec. classes
1050  set-precipitation-parameter zet_p4 nucleation-parent-precipitate=vn_p4 $ nucleation
      sites are existing VN prec.
1051  set-precipitation-parameter zet_p4 equivalent-interface-energy=eie_zet $ use equiv.
      intf. energy
1052  set-precipitation-parameter zet_p4 nucleation-model=particle-related-transformation
      $ use direct particle transf. nucl. model
1053  set-precipitation-parameter ZET_P4
      restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
      precipitation domain
1054  set-precipitation-parameter ZET_P4 minimum-nucleation-radius=zmnr
```

Figure A.28.: MatCalc-script: Precipitation kinetics (p.24)

```
1055
1056   create-new-phase parent-phase=ZET precipitate Z(mart,vn_m_sgb) $ new prec. phase for
       Zet-phase in martensite
1057   set-precipitation-parameter zet_p5 number-of-size-classes=npc_z $ use variable for
       prec. classes
1058   set-precipitation-parameter zet_p5 nucleation-parent-precipitate=vn_p5 $ nucleation
       sites are existing VN prec.
1059   set-precipitation-parameter zet_p5 equivalent-interface-energy=eie_zet $ use equiv.
       intf. energy
1060   set-precipitation-parameter zet_p5 nucleation-model=particle-related-transformation
       $ use direct particle transf. nucl. model
1061   set-precipitation-parameter ZET_P5
       restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
       precipitation domain
1062   set-precipitation-parameter ZET_P5 minimum-nucleation-radius=zmnr
1063
1064   $ Zet-phase can also nucleate directly from the matrix. However, its nuclei with
       rather complex
1065   $ crystal structure is in direct competition with the MX phase with simple fcc. For
       that reason,
1066   $ the probability of Z-phase nucleation is extremely low, because Cr, V and N will
       nucleate the simple
1067   $ structure much easier than the double-layer structure of Zet. Estimates
       (Sonderegger/Danielsen/
1068   $ Kozeschnik, 2005, unpublished) deliver a factor of 1e-12. This value is entered as
       nucleation
1069   $ constant, to reflect this competitive (entropic) effect
1070
1071   create-new-phase parent-phase=ZET precipitate Z(matrix,di) $ new prec. phase for
       Zet-phase in martensite
1072   set-precipitation-parameter zet_p6 number-of-size-classes=npc_z $ use variable for
       prec. classes
1073   set-precipitation-parameter zet_p6 nucleation-sites=dislocations $ nucleation sites
       are dislocation
1074   set-precipitation-parameter zet_p6 nucleation-constant=nucl_const_zet $ nucleation
       constant for matrix Z-phase
1075   set-precipitation-parameter ZET_P6
       restrict-nucleation-to-precipitation-domain=martensite $ restrict nucleation to
       precipitation domain
1076   set-precipitation-parameter ZET_P6 minimum-nucleation-radius=zmnr
1077
1078
1079   $ + + + + + OUTPUT WINDOWS, PLOTS, ETC.
1080
1081   if (userselection==3)
1082   else
1083
1084   new-gui-window type-id=p1 $ generate new plot: Hardening
1085   set-variable-value variable=window_id_hardening value=active_frame_id $ save windows
       id to variable
1086
1087   set-gui-window-property window-id=. default-x-axis-data=stepvalue $ default x-axis
       variable (time)
1088   set-gui-window-property window-id=. default-x-axis-for-all-plots=yes $ use default
       x-axis for all plots: yes
1089   set-gui-window-property window-id=. default-x-axis-title=time [min] $ default x-axis
       title
1090   set-gui-window-property window-id=. default-x-axis-factor=1/60 $ scaling factor is
       1/60 for min
1091   set-gui-window-property window-id=. number-of-plot-columns=2 $ 2 plot columns
1092
1093   set-plot-option plot-id=. series new buffer t$c $ add series: temperature
1094   set-plot-option plot-id=. series rename series-index=-1 series-name=t$c new-name=T $
       define series legend
1095   set-plot-option plot-id=. y-axis-title=temperature [°C] $ y-axis title
1096
1097   format-variable-string variable=title1 format-string="%s_%s" #samplename Hardening
1098   set-plot-option plot-id=. plot-title=#title1 $ define plot title
1099
```

Figure A.29.: MatCalc-script: Precipitation kinetics (p.25)

```
1100  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: phase
      fractions
1101  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1102  set-plot-option plot-id=. series new buffer f_prec$* $ add all series: phase
      fractions of prec.
1103  set-plot-option plot-id=. y-axis-title=phase fraction [%] $ y-axis title
1104  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1105  set-plot-option plot-id=. y-axis-factor=100 $ scaling factor is 100 for percent
1106  set-plot-option plot-id=. y-axis-scaling=1e-4.. $ scale the y-axis from 1e-4..
1107
1108  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: mean diameter
1109  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1110  set-plot-option plot-id=. series new buffer d_mean$* $ add all series: mean diameter
      of precipitates
1111  set-plot-option plot-id=. y-axis-title=mean diameter [nm] $ change y-axis title
1112  set-plot-option plot-id=. y-axis-type=lin $ use linear scale for y-axis
1113  set-plot-option plot-id=. y-axis-factor=1e9 $ scaling factor is 1e9 for nm
1114
1115  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: number
      densities
1116  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace all variable names
      by kinetic alias
1117  set-plot-option plot-id=. series new buffer num_part$* $ add all series: number
      densities of precipitates
1118  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>] $ change
      y-axis title
1119  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1120  set-plot-option plot-id=. y-axis-scaling=1e10.. $ scale the y-axis from 1e10..
1121
1122  move-gui-window displace window-id=. x-origin=50 y-origin=10 width=700 height=950 $
      move window to new position and resize
1123  update-gui-window window-id=. $ update the GUI window
1124  move-gui-window hide window-id=. $ hide plot
1125
1126  new-gui-window type-id=p1 $ generate new plot: Tempering
1127  set-variable-value variable=window_id_tempering value=active_frame_id $ save windows
      id to variable
1128
1129  set-gui-window-property window-id=. default-x-axis-data=stepvalue $ default x-axis
      variable (time)
1130  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes $ use default
      x-axis for all plots: yes
1131  set-gui-window-property window-id=. default-x-axis-title=time [min] $ default x-axis
      title
1132  set-gui-window-property window-id=. default-x-axis-factor=1/60 $ scaling factor is
      1/60 for min
1133  set-gui-window-property window-id=. number-of-plot-columns=2 $ 2 plot columns
1134
1135  set-plot-option plot-id=. series new buffer t$c $ add series: temperature
1136  set-plot-option plot-id=. series rename series-index=-1 series-name=t$c new-name=T $
      define series legend
1137  set-plot-option plot-id=. y-axis-title=temperature [°C] $ y-axis title
1138
1139  format-variable-string variable=title2 format-string="%s_%s" #samplename Tempering
1140  set-plot-option plot-id=. plot-title=#title2 $ define plot title
1141
1142  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: phase
      fractions
1143  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1144  set-plot-option plot-id=. series new buffer f_prec$* $ add all series: phase
      fractions of prec.
1145  set-plot-option plot-id=. y-axis-title=phase fraction [%] $ y-axis title
1146  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1147  set-plot-option plot-id=. y-axis-factor=100 $ scaling factor is 100 for percent
1148  set-plot-option plot-id=. y-axis-scaling=1e-4.. $ scale the y-axis from 1e-4..
1149
```

Figure A.30.: MatCalc-script: Precipitation kinetics (p.26)

```
1150  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: mean diameter
1151  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1152  set-plot-option plot-id=. series new buffer d_mean$* $ add all series: mean diameter
      of precipitates
1153  set-plot-option plot-id=. y-axis-title=mean diameter [nm] $ change y-axis title
1154  set-plot-option plot-id=. y-axis-type=lin $ use linear scale for y-axis
1155  set-plot-option plot-id=. y-axis-factor=1e9 $ scaling factor is 1e9 for nm
1156
1157  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: number
      densities
1158  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace all variable names
      by kinetic alias
1159  set-plot-option plot-id=. series new buffer num_part$* $ add all series: number
      densities of precipitates
1160  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>] $ change
      y-axis title
1161  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1162  set-plot-option plot-id=. y-axis-scaling=1e10.. $ scale the y-axis from 1e10..
1163
1164  move-gui-window displace window-id=. x-origin=70 y-origin=10 width=700 height=950 $
      move window to new position and resize
1165  update-gui-window window-id=. $ update the GUI window
1166  move-gui-window hide window-id=. $ hide plot
1167
1168  endif
1169
1170  $ execute following part for welding/fghaz
1171
1172  if (userselection==1)
1173  else
1174
1175  new-gui-window type-id=p1 $ generate new plot: Welding
1176  set-variable-value variable=window_id_welding value=active_frame_id $ save windows
      id to variable
1177
1178  set-gui-window-property window-id=. default-x-axis-data=stepvalue $ default x-axis
      variable (time)
1179  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes $ use default
      x-axis for all plots: yes
1180  set-gui-window-property window-id=. default-x-axis-title=time [min] $ default x-axis
      title
1181  set-gui-window-property window-id=. default-x-axis-factor=1/60 $ scaling factor is
      1/60 for min
1182  set-gui-window-property window-id=. number-of-plot-columns=2 $ 2 plot columns
1183
1184  set-plot-option plot-id=. series new buffer t$c $ add series: temperature
1185  set-plot-option plot-id=. series rename series-index=-1 series-name=t$c new-name=T $
      define series legend
1186  set-plot-option plot-id=. y-axis-title=temperature [°C] $ y-axis title
1187
1188  format-variable-string variable=title3 format-string="%s_%s" #samplename Welding
1189  set-plot-option plot-id=. plot-title=#title3 $ define plot title
1190
1191  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: phase
      fractions
1192  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1193  set-plot-option plot-id=. series new buffer f_prec$* $ add all series: phase
      fractions of prec.
1194  set-plot-option plot-id=. y-axis-title=phase fraction [%] $ y-axis title
1195  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1196  set-plot-option plot-id=. y-axis-factor=100 $ scaling factor is 100 for percent
1197  set-plot-option plot-id=. y-axis-scaling=1e-4.. $ scale the y-axis from 1e-4..
1198
1199  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: mean diameter
1200  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1201  set-plot-option plot-id=. series new buffer d_mean$* $ add all series: mean diameter
```

Figure A.31.: MatCalc-script: Precipitation kinetics (p.27)

```
      of precipitates
1202  set-plot-option plot-id=. y-axis-title=mean diameter [nm] $ change y-axis title
1203  set-plot-option plot-id=. y-axis-type=lin $ use linear scale for y-axis
1204  set-plot-option plot-id=. y-axis-factor=1e9 $ scaling factor is 1e9 for nm
1205
1206  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: number
      densities
1207  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace all variable names
      by kinetic alias
1208  set-plot-option plot-id=. series new buffer num_part$* $ add all series: number
      densities of precipitates
1209  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>] $ change
      y-axis title
1210  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1211  set-plot-option plot-id=. y-axis-scaling=1e10.. $ scale the y-axis from 1e10..
1212
1213  move-gui-window displace window-id=. x-origin=90 y-origin=10 width=700 height=950 $
      move window to new position and resize
1214  update-gui-window window-id=. $ update the GUI window
1215  move-gui-window hide window-id=. $ hide plot
1216
1217
1218  new-gui-window type-id=p1 $ generate new plot: PWHT
1219  set-variable-value variable=window_id_pwht value=active_frame_id $ save windows id
      to variable
1220
1221  set-gui-window-property window-id=. default-x-axis-data=stepvalue $ default x-axis
      variable (time)
1222  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes $ use default
      x-axis for all plots: yes
1223  set-gui-window-property window-id=. default-x-axis-title=time [min] $ default x-axis
      title
1224  set-gui-window-property window-id=. default-x-axis-factor=1/60 $ scaling factor is
      1/60 for min
1225  set-gui-window-property window-id=. number-of-plot-columns=2 $ 2 plot columns
1226
1227  set-plot-option plot-id=. series new buffer t$c $ add series: temperature
1228  set-plot-option plot-id=. series rename series-index=-1 series-name=t$c new-name=T $
      define series legend
1229  set-plot-option plot-id=. y-axis-title=temperature [°C] $ y-axis title
1230
1231  format-variable-string variable=title4 format-string="%s_%s" #samplename PWHT
1232  set-plot-option plot-id=. plot-title=#title4 $ define plot title
1233
1234  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: phase
      fractions
1235  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1236  set-plot-option plot-id=. series new buffer f_prec$* $ add all series: phase
      fractions of prec.
1237  set-plot-option plot-id=. y-axis-title=phase fraction [%] $ y-axis title
1238  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1239  set-plot-option plot-id=. y-axis-factor=100 $ scaling factor is 100 for percent
1240  set-plot-option plot-id=. y-axis-scaling=1e-4.. $ scale the y-axis from 1e-4..
1241
1242  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: mean diameter
1243  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1244  set-plot-option plot-id=. series new buffer d_mean$* $ add all series: mean diameter
      of precipitates
1245  set-plot-option plot-id=. y-axis-title=mean diameter [nm] $ change y-axis title
1246  set-plot-option plot-id=. y-axis-type=lin $ use linear scale for y-axis
1247  set-plot-option plot-id=. y-axis-factor=1e9 $ scaling factor is 1e9 for nm
1248
1249  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: number
      densities
1250  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace all variable names
      by kinetic alias
1251  set-plot-option plot-id=. series new buffer num_part$* $ add all series: number
```

Figure A.32.: MatCalc-script: Precipitation kinetics (p.28)

```
      densities of precipitates
1252  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>] $ change
      y-axis title
1253  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1254  set-plot-option plot-id=. y-axis-scaling=1e10.. $ scale the y-axis from 1e10..
1255
1256  move-gui-window displace window-id=. x-origin=110 y-origin=10 width=700 height=950 $
      move window to new position and resize
1257  update-gui-window window-id=. $ update the GUI window
1258  move-gui-window hide window-id=. $ hide plot
1259
1260  endif
1261
1262  new-gui-window type-id=p1 $ generate new plot: Service
1263  set-variable-value variable=window_id_service value=active_frame_id $ save windows
      id to variable
1264
1265  set-gui-window-property window-id=. default-x-axis-data=stepvalue $ default x-axis
      variable (time)
1266  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes $ use default
      x-axis for all plots: yes
1267  set-gui-window-property window-id=. default-x-axis-title=time [h] $ default x-axis
      title
1268  set-gui-window-property window-id=. default-x-axis-factor=1/3600 $ scaling factor is
      1/60 for min
1269  set-gui-window-property window-id=. number-of-plot-columns=2 $ 2 plot columns
1270
1271  set-plot-option plot-id=. series new buffer t$c $ add series: temperature
1272  set-plot-option plot-id=. series rename series-index=-1 series-name=t$c new-name=T $
      define series legend
1273  set-plot-option plot-id=. y-axis-title=temperature [°C] $ y-axis title
1274
1275  format-variable-string variable=title5 format-string="%s_%s" #samplename Service
1276  set-plot-option plot-id=. plot-title=#title5 $ define plot title
1277
1278  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: phase
      fractions
1279  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1280  set-plot-option plot-id=. series new buffer f_prec$* $ add all series: phase
      fractions of prec.
1281  set-plot-option plot-id=. y-axis-title=phase fraction [%] $ y-axis title
1282  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1283  set-plot-option plot-id=. y-axis-factor=100 $ scaling factor is 100 for percent
1284  set-plot-option plot-id=. y-axis-scaling=1e-4.. $ scale the y-axis from 1e-4..
1285
1286  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: mean diameter
1287  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace variable names by
      kinetic alias
1288  set-plot-option plot-id=. series new buffer d_mean$* $ add all series: mean diameter
      of precipitates
1289  set-plot-option plot-id=. y-axis-title=mean diameter [nm] $ change y-axis title
1290  set-plot-option plot-id=. y-axis-type=lin $ use linear scale for y-axis
1291  set-plot-option plot-id=. y-axis-factor=1e9 $ scaling factor is 1e9 for nm
1292
1293  create-new-plot plot-type=xy-plot attach-to-window=. $ create new plot: number
      densities
1294  set-plot-option plot-id=. use-alias-names-in-legend=yes $ replace all variable names
      by kinetic alias
1295  set-plot-option plot-id=. series new buffer num_part$* $ add all series: number
      densities of precipitates
1296  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>] $ change
      y-axis title
1297  set-plot-option plot-id=. y-axis-type=log $ use logarithmic scale for y-axis
1298  set-plot-option plot-id=. y-axis-scaling=1e10.. $ scale the y-axis from 1e10..
1299
1300  move-gui-window displace window-id=. x-origin=130 y-origin=10 width=700 height=950 $
      move window to new position and resize
1301  update-gui-window window-id=. $ update the GUI window
```

Figure A.33.: MatCalc-script: Precipitation kinetics (p.29)

```
1302  move-gui-window hide window-id=. $ hide plot
1303
1304
1305  $ + + + + + HISTOGRAMM + + + + +
1306
1307
1308  new-gui-window type-id=p5                                          $ new
      precipitation distribution plot window
1309  set-gui-window-property window-id=. number-of-plot-columns=2
1310  set-gui-window-property window-id=. default-x-axis-for-all-plots=yes
1311  set-gui-window-property window-id=. default-x-axis-title=diameter [nm]
1312  set-gui-window-property window-id=. default-x-axis-factor=2e9              $ factor
      for nanometer and diameter instead of radius
1313  set-gui-window-property window-id=. default-x-axis-type=log
1314  set-gui-window-property window-id=. default-x-axis-scaling=1..10000
1315
1316  set-plot-option plot-id=. use-alias-names-in-legend=yes                    $
      replace variable names by kinetic alias
1317  set-plot-option plot-id=. series new precipitate-distribution VN_p0
1318  set-plot-option plot-id=. series new precipitate-distribution VN_p1
1319  set-plot-option plot-id=. series new precipitate-distribution VN_p2
1320  set-plot-option plot-id=. series new precipitate-distribution VN_p3
1321  set-plot-option plot-id=. series new precipitate-distribution VN_p4
1322  set-plot-option plot-id=. series new precipitate-distribution VN_p5
1323  set-plot-option plot-id=. y-axis-scaling=#scale_range
1324  set-plot-option plot-id=. y-axis-type=log                                  $ use
      logarithmic scale for y-axis
1325  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>]
1326
1327  create-new-plot plot-type=precipitate-distribution attach-to-window=.     $ create
      new plot: precipitate distribution
1328  set-plot-option plot-id=. use-alias-names-in-legend=yes
1329  set-plot-option plot-id=. series new precipitate-distribution NbC_p0
1330  set-plot-option plot-id=. series new precipitate-distribution NbC_p1
1331  set-plot-option plot-id=. series new precipitate-distribution NbC_p2
1332  set-plot-option plot-id=. series new precipitate-distribution NbC_p3
1333  set-plot-option plot-id=. series new precipitate-distribution NbC_p4
1334  set-plot-option plot-id=. series new precipitate-distribution NbC_p5
1335  set-plot-option plot-id=. y-axis-scaling=#scale_range
1336  set-plot-option plot-id=. y-axis-type=log
1337  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>]
1338
1339  create-new-plot plot-type=precipitate-distribution
      attach-to-window=.
1340  set-plot-option plot-id=. use-alias-names-in-legend=yes
1341  set-plot-option plot-id=. series new precipitate-distribution AlN_p0
1342  set-plot-option plot-id=. series new precipitate-distribution AlN_p1
1343  set-plot-option plot-id=. y-axis-scaling=#scale_range
1344  set-plot-option plot-id=. y-axis-type=log
1345  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup
1346
1347  create-new-plot plot-type=precipitate-distribution attach-to-window=.
1348  set-plot-option plot-id=. use-alias-names-in-legend=yes
1349  set-plot-option plot-id=. series new precipitate-distribution Cr2N_p0
1350  set-plot-option plot-id=. series new precipitate-distribution Cr2N_p1
1351  set-plot-option plot-id=. series new precipitate-distribution Cr2N_p2
1352  set-plot-option plot-id=. series new precipitate-distribution cementite_p0
1353  set-plot-option plot-id=. series new precipitate-distribution cementite_p1
1354  set-plot-option plot-id=. series new precipitate-distribution cementite_p2
1355  set-plot-option plot-id=. y-axis-scaling=#scale_range
1356  set-plot-option plot-id=. y-axis-type=log
1357  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>]
1358
1359  create-new-plot plot-type=precipitate-distribution attach-to-window=.
1360  set-plot-option plot-id=. use-alias-names-in-legend=yes
1361  set-plot-option plot-id=. series new precipitate-distribution Laves_phase_p0
1362  set-plot-option plot-id=. series new precipitate-distribution Laves_phase_p1
1363  set-plot-option plot-id=. y-axis-scaling=#scale_range
1364  set-plot-option plot-id=. y-axis-type=log
```

Figure A.34.: MatCalc-script: Precipitation kinetics (p.30)

```
1365  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>]
1366
1367  create-new-plot plot-type=precipitate-distribution
      attach-to-window=.
1368  set-plot-option plot-id=. use-alias-names-in-legend=yes
1369  set-plot-option plot-id=. series new precipitate-distribution m7c3_p0
1370  set-plot-option plot-id=. series new precipitate-distribution m7c3_p1
1371  set-plot-option plot-id=. series new precipitate-distribution m7c3_p2
1372  set-plot-option plot-id=. y-axis-scaling=#scale_range
1373  set-plot-option plot-id=. y-axis-type=log
1374  set-plot-option plot-id=. y-axis-title=number density
      [m<sup>-3</sup>]
1375
1376  create-new-plot plot-type=precipitate-distribution
      attach-to-window=.
1377  set-plot-option plot-id=. use-alias-names-in-legend=yes
1378  set-plot-option plot-id=. series new precipitate-distribution m23c6_p0
1379  set-plot-option plot-id=. series new precipitate-distribution m23c6_p1
1380  set-plot-option plot-id=. series new precipitate-distribution m23c6_p2
1381  set-plot-option plot-id=. y-axis-scaling=#scale_range
1382  set-plot-option plot-id=. y-axis-type=log
1383  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>]
1384
1385  create-new-plot plot-type=precipitate-distribution attach-to-window=.
1386  set-plot-option plot-id=. use-alias-names-in-legend=yes
1387  set-plot-option plot-id=. series new precipitate-distribution zet_p0
1388  set-plot-option plot-id=. series new precipitate-distribution zet_p1
1389  set-plot-option plot-id=. series new precipitate-distribution zet_p2
1390  set-plot-option plot-id=. series new precipitate-distribution zet_p3
1391  set-plot-option plot-id=. series new precipitate-distribution zet_p4
1392  set-plot-option plot-id=. series new precipitate-distribution zet_p5
1393  set-plot-option plot-id=. series new precipitate-distribution zet_p6
1394  set-plot-option plot-id=. y-axis-scaling=#scale_range
1395  set-plot-option plot-id=. y-axis-type=log
1396  set-plot-option plot-id=. y-axis-title=number density [m<sup>-3</sup>]
1397
1398  move-gui-window displace window-id=. x-origin=135 y-origin=10 width=750 height=700
1399  update-gui-window window-id=.     $ update the GUI window
1400
1401
1402  $ + + + + + START PRECIPITATE SIMULATION + + + + +
1403
1404  $ speed up simulations, modify numerical parameters
1405  set-simulation-parameter max-radius-change-during-growth=1
1406  set-simulation-parameter update-every=1000
1407
1408  if (userselection==3)
1409  else
1410
1411  $ START PRECIPITATE SIMULATION PART HARDENING
1412
1413  create-calc-buffer new-buffer-name=hardening $ rename buffer for heat treatment
1414  set-gui-window-property window-id=window_id_hardening buffer-name=hardening $ attach
      to buffer window
1415  move-gui-window show window-id=window_id_hardening $ bring plot to front
1416
1417  set-simulation-parameter temperature-control-type=from-tm-treatment
1418  set-simulation-parameter tm-treatment-name=hardening
1419  set-simulation-parameter starting-conditions=reset-precipitates
1420
1421  start-precipitate-simulation $ calculate part hardening
1422
1423  $ save state after simulation. Is starting point for next simulation part II
1424  create-calc-state new-state-name=after_hardening
1425
1426
1427  $ START PRECIPITATE SIMULATION PART TEMPERING
1428
1429  create-calc-buffer new-buffer-name=tempering $ create buffer for HT
```

Figure A.35.: MatCalc-script: Precipitation kinetics (p.31)

```
1430  select-calc-buffer buffer-name=tempering $ select calc buffer
1431  set-gui-window-property window-id=window_id_tempering buffer-name=tempering $ attach
      to buffer window
1432  move-gui-window show window-id=window_id_tempering $ bring plot to front
1433
1434  set-simulation-parameter temperature-control-type=from-tm-treatment
1435  set-simulation-parameter tm-treatment-name=tempering
1436  set-simulation-parameter starting-conditions=after_hardening
1437
1438  start-precipitate-simulation $ calculate part tempering
1439
1440  $ save state after simulation. Is starting point for next simulation part III
1441  create-calc-state new-state-name=after_tempering
1442
1443  endif
1444
1445
1446  $ execute following part for FGHAZ
1447  $ START PRECIPITATE SIMULATION PART WELDING
1448  if (userselection==1)
1449  else
1450
1451  create-calc-buffer new-buffer-name=welding $ create buffer for HT
1452  select-calc-buffer buffer-name=welding $ select calc buffer
1453  set-gui-window-property window-id=window_id_welding buffer-name=welding $ attach to
      buffer window
1454  move-gui-window show window-id=window_id_welding $ bring plot to front
1455
1456  set-simulation-parameter temperature-control-type=from-tm-treatment
1457  set-simulation-parameter tm-treatment-name=welding
1458  endif
1459
1460  if (userselection==2)
1461  set-simulation-parameter starting-conditions=after_tempering
1462  elseif (userselection==3)
1463  set-simulation-parameter starting-conditions=reset-precipitates
1464  endif
1465
1466  if (userselection==1)
1467  else
1468  start-precipitate-simulation $ calculate part welding
1469
1470  $ save state after simulation. Is starting point for next simulation part IV
1471  create-calc-state new-state-name=after_welding
1472
1473  $ relic code from 5.61, maybe useful for later sometimes
1474
1475  $ increase matrix diffusion enhancement factor to 8 before start of PWHT
1476  $set-precipitation-parameter nbc_p0 s m s mdef $ individual matrix diff. enh. factor
1477  $set-precipitation-parameter nbc_p1 s m s mdef $ individual matrix diff. enh. factor
1478  $set-precipitation-parameter nbc_p2 s m s mdef $ individual matrix diff. enh. factor
1479  $set-precipitation-parameter nbc_p3 s m s mdef $ individual matrix diff. enh. factor
1480  $set-precipitation-parameter nbc_p4 s m s mdef $ individual matrix diff. enh. factor
1481  $set-precipitation-parameter aln_p0 s m s mdef $ individual matrix diff. enh. factor
1482  $set-precipitation-parameter aln_p1 s m s mdef $ individual matrix diff. enh. factor
1483  $set-precipitation-parameter cr2n_p0 s m s mdef $ individual matrix diff. enh.
      factor
1484  $set-precipitation-parameter cr2n_p1 s m s mdef $ individual matrix diff. enh.
      factor
1485  $set-precipitation-parameter vn_p0 s m s mdef $ individual matrix diff. enh. factor
1486  $set-precipitation-parameter vn_p1 s m s mdef $ individual matrix diff. enh. factor
1487  $set-precipitation-parameter vn_p2 s m s mdef $ individual matrix diff. enh. factor
1488  $set-precipitation-parameter vn_p3 s m s mdef $ individual matrix diff. enh. factor
1489  $set-precipitation-parameter m23c6_p0 s m s mdef $ individual matrix diff. enh.
      factor
1490  $set-precipitation-parameter m23c6_p1 s m s mdef $ individual matrix diff. enh.
      factor
1491  $set-precipitation-parameter m7c3_p0 s m s mdef $ individual matrix diff. enh.
      factor
```

Figure A.36.: MatCalc-script: Precipitation kinetics (p.32)

```
1492  $set-precipitation-parameter cementite_p0 s m s mdef $ individual matrix diff. enh.
      factor
1493  $set-precipitation-parameter laves_phase_p0 s m s mdef $ individual matrix diff.
      enh. factor
1494  $set-precipitation-parameter zet_p0 s m s mdef $ individual matrix diff. enh. factor
1495  $set-precipitation-parameter zet_p1 s m s mdef $ individual matrix diff. enh. factor
1496  $set-precipitation-parameter zet_p2 s m s mdef $ individual matrix diff. enh. factor
1497  $set-precipitation-parameter zet_p3 s m s mdef $ individual matrix diff. enh. factor
1498  $set-precipitation-parameter zet_p4 s m s mdef $ individual matrix diff. enh. factor
1499
1500
1501  $ START PRECIPITATE SIMULATION PWHT
1502  create-calc-buffer new-buffer-name=pwht $ create buffer for HT
1503  select-calc-buffer buffer-name=pwht $ select calc buffer
1504  set-gui-window-property window-id=window_id_pwht buffer-name=pwht $ attach to buffer
      window
1505  move-gui-window show window-id=window_id_pwht $ bring plot to front
1506
1507  set-simulation-parameter temperature-control-type=from-tm-treatment
1508  set-simulation-parameter tm-treatment-name=pwht
1509  set-simulation-parameter starting-conditions=after_welding
1510
1511  start-precipitate-simulation $ calculate part 4, post weld heat treatment
1512
1513  $ save state after simulation. Is starting point for next simulation part V
1514  create-calc-state new-state-name=after_pwht
1515
1516  endif
1517
1518  $ START PRECIPITATE SIMULATION SERVICE
1519  create-calc-buffer new-buffer-name=service $ create buffer for HT
1520  select-calc-buffer buffer-name=service $ select calc buffer
1521  set-gui-window-property window-id=window_id_service buffer-name=service $ attach to
      buffer window
1522  move-gui-window show window-id=window_id_service $ bring plot to front
1523
1524  set-simulation-parameter temperature-control-type=from-tm-treatment
1525  set-simulation-parameter tm-treatment-name=service
1526  set-simulation-parameter max-temperature-step=1
1527
1528  if (userselection==1)
1529  set-simulation-parameter starting-conditions=after_tempering
1530  else
1531  set-simulation-parameter starting-conditions=after_pwht
1532  endif
1533
1534  start-precipitate-simulation $ calculate service conditions
1535
1536  $ save state after simulation.
1537  create-calc-state new-state-name=after_service
1538
1539  $ + + + + + PRECIPITATE SIMULATION FINISHED + + + + +
1540
1541
1542  $ compose name variable for workspace-name
1543  if (userselection==1)
1544  format-variable-string variable=workspacename format-string="%s_%s_%s_%d" #version
      #samplename BM #T_serv
1545  elseif (userselection==2)
1546  format-variable-string variable=workspacename format-string="%s_%s_%s_%d" #version
      #samplename FGHAZ #T_serv
1547  elseif (userselection==3)
1548  format-variable-string variable=workspacename format-string="%s_%s_%s_%d" #version
      #samplename WELD #T_serv
1549  else
1550  endif
1551
1552  save-workspace #workspacename
```

Figure A.37.: MatCalc-script: Precipitation kinetics (p.33)

Appendix B.

Scripts Matlab

creep_model_start.m 1 of 2

```
%%
% *_Creep Model_* according to "Modelling the creep behaviour
% of tempered martensitic steel based on a hybrid approach" with
% improvements in model and script.
%
% Copyright 2018
% Yadav, Krenmayr, Sonderegger, Riedlsperger, Schmid, Fercher

%% Test conditions and related creep data

% Clearing all variables except time_to_rupture_diagram_matrix to avoid
% potential errors

clearvars % -except time_to_rupture_diagram_matrix

script_version = 'Matlab Creep Model v2.0';

%% open subfile for service conditions
settings

%start progressbar
f = waitbar(0,'loading experimental data and settings ...',...
    'Name',script_version);
loop_counter = 0; % loop counter for progress bar

%% import of experimental Data
experimental_data

%% General parameter settings

% Boltzmann constant
k = physconst('Boltzmann');

% maximum simulation hours [h]
TIME_MAX = max(CreepData(:,1))*3600;

% timestep [s]
TIME_STEP = 1;

% Calculation of the iterations
NUMBER_OF_ITERATIONS = 1e6;
%TODO Find better/best value for number of iterations

% Convert from °C to K [after settings.m]
T = T+273.15;

%% Preload model-parameter-excel-file outside the loop once
filename_parameters = 'exp_parameters.xlsx';
micro_parameters = xlsread(filename_parameters,exp_tab_name,'C3:C25');
mod_parameters = xlsread(filename_parameters,exp_tab_name,'H3:H30');

%% Load and process Matcalc-data if selected previously
if matcalc_choice == 1
   process_matcalc_data
end

%% MAIN calculation loop for all selected applied stress levels

for i=1:sigma_applied_steps

%load parameters
parameters

```

Figure B.1.: Matlab-script: Creep model start (p.1)

```
64 % Main model
65 main_model
66
67 % Data visualisation
68 plot_figures
69
70 end
71
72 %% Plot Time to rupture diagram
73
74 time_to_rupture_diagram
75
```

Figure B.2.: Matlab-script: Creep model start (p.2)

settings.m 1 of 2

```
%% Dialog window, for chosing some calculation options

prompt1 = {"BASIC MODEL CHOICES:" + newline + newline + ...
    "Use Matcalc data? [1] or [0]",...
    'Use effective velocity v_eff for mobile dislocations? [1] or [0]',...
    'Calculation with Damage? (Modified Orowan equation) [1] or [0]',...
    'Percent change per time step [%]',newline + ...
    "EXPERIMENTAL DATA SOURCES:" + newline + newline + ...
    "MatCalc precipitates datasets",...
    'Fitparameter dataset', ...
    "Creep curve comparision dataset",newline + ...
    "SERVICE CONDITIONS:" + newline + newline + ...
    "Creep temperature [°C]",...
    'Applied Stress maximum [MPa]',...
    'Applied Stress minimum [MPa]',...
    'Number of stress curves to calculate [ ]'};
dlg_title1 = 'Matlab Creep Model v2.0';
num_lines1 = 0.35;

% choices_default = {'1','1','1','0.1','BM-650-Schmid',...
%    'BM-650C-80MPa-BF','BM-650C-80MPa','650','110','50','7'};
% Literature

% choices_default = {'1','1','1','0.1','WELD-600-Fercher',...
%   'MgC-600C-130MPa-BF','MgC-600C-130MPa','600','160','100','7'};
% Fit tof MgC 600 -Literature

% choices_default = {'1','1','1','0.1','WELD-625-Fercher',...
%   'WELD-625C-BF','MgC-600C-130MPa','625','130','70','7'};
% no literature creep curve for 625°C

 choices_default = {'1','1','1','0.1','WELD-600-Fercher',...
   'WELD-600C-BF','MgC-600C-130MPa','600','160','100','7'};
% Fit to WELD 600

%choices_default = {'1','1','1','0.1','WELD-575-Fercher',...
%     'WELD-575C-BF','MgC-600C-130MPa','575','190','130','7'};
% no literature creep curve for 575°C

%choices_default = {'0','0','1','0.1','BM-650-Schmid',...
%    'BM-650C-80MPa-BF','BM-650C-80MPa','650','110','50','7'};
% for quick testing of code and graphics


% Open the input dialog window
choices_selected = inputdlg(prompt1,dlg_title1,num_lines1,choices_default);


%% put selections into single variables

% Calculation options
matcalc_choice = sscanf(sprintf('%s',choices_selected{1,1}),'%f*');
v_eff_choice = sscanf(sprintf('%s',choices_selected{2,1}),'%f*');
damage_choice = sscanf(sprintf('%s',choices_selected{3,1}),'%f*');

% Allowed percentage change, each time step
percentage_change = sscanf(sprintf('%s',choices_selected{4,1}),'%f*');

% Experimental data for different applied stresses [MPa]
MatCalc_tab_name = choices_selected{5,1};
exp_tab_name = choices_selected{6,1};
creep_tab_name = choices_selected{7,1};

```

Figure B.3.: Matlab-script: Creep model settings (p.1)

```
64 % Service temperature [°C]
65 T = sscanf(sprintf('%s',choices_selected{8,1}),'%f*');
66
67 % Applied stress starting point [MPa]
68 sigma_applied_start = sscanf(sprintf('%s',choices_selected{9,1}),'%f*');
69
70 % Applied stress range and number of intervals
71 sigma_applied_end = sscanf(sprintf('%s',choices_selected{10,1}),'%f*');
72 sigma_applied_steps = sscanf(sprintf('%s',choices_selected{11,1}),'%f*');
73
74 % Some explanations of the dialog windows
75 if v_eff_choice == 1 && matcalc_choice == 0
76     matcalc = 1;
77     disp('Error: To calculate v_eff, MatCalc data is necessary');
78     disp('Error: MatCalc data will be used to calculate v_eff');
79 end
80
81 % variable splitting to preserve the stress value in [MPa] for model
82 sigma_applied_stepper = sigma_applied_start;
83
```

Figure B.4.: Matlab-script: Creep model settings (p.2)

experimental_data.m 1 of 1

```
%% LEGACY CODE
% Create the correct file- and spreadsheetname
% spreadsheetname = [sscanf(sprintf('%s',exp_data_name),'%s'),...
%     '_',sprintf('%d',T),'C_',sprintf('%d',sigma_applied_exp),'MPa'];
%diagramtitle = [sscanf(sprintf('%s',exp_tab_name),'%s'),...
%    ' / ',sprintf('%d',T),'C / ',sprintf('%d',exp_tab_name),'MPa'];

%% Import and process experimental data
% Import the data from the Excel-file
filename_creep_data = 'exp_creep_curves.xlsx';
CreepData = xlsread(filename_creep_data,creep_tab_name,'C10:D5000');

% Smoothing of creep data (bad when working with few points)
% CreepData(:,2) = smooth(CreepData(:,2),5);

% Erase all creep data with more than 6% elongation
CreepData(CreepData(:,2)>6,:)=[];

% Evaluate the maximum time of the experimental data
rup_time_exp = max(CreepData(:,1));

%% Import the data for the time to rupture diagrams from the Excel-file

fn_ttr_data = 'exp_rupture_data.xlsx';

% ttr_data_NIMS = xlsread(fn_ttr_data,'NIMS','A2:B6');
ttr_data_ECCC = xlsread(fn_ttr_data,'ECCC','A2:B44');
ttr_data_ASME = xlsread(fn_ttr_data,'ASME','A2:B7');

ttr_data_NIMS_650_MgA = xlsread(fn_ttr_data,'NIMS-650','A2:B6');
ttr_data_NIMS_650_MgB = xlsread(fn_ttr_data,'NIMS-650','A12:B17');
ttr_data_NIMS_650_MgC = xlsread(fn_ttr_data,'NIMS-650','A22:B26');

ttr_data_NIMS_600_MgA = xlsread(fn_ttr_data,'NIMS-600','A2:B6');
ttr_data_NIMS_600_MgB = xlsread(fn_ttr_data,'NIMS-600','A12:B17');
ttr_data_NIMS_600_MgC = xlsread(fn_ttr_data,'NIMS-600','A22:B26');

ttr_data_NIMS_550_MgA = xlsread(fn_ttr_data,'NIMS-550','A2:B6');
ttr_data_NIMS_550_MgB = xlsread(fn_ttr_data,'NIMS-550','A12:B17');
ttr_data_NIMS_550_MgC = xlsread(fn_ttr_data,'NIMS-550','A22:B26');

ttr_data_Hxx_575 = xlsread(fn_ttr_data,'Boehler','C4:D8');
ttr_data_Hxx_600 = xlsread(fn_ttr_data,'Boehler','C10:D15');
ttr_data_Hxx_625 = xlsread(fn_ttr_data,'Boehler','C17:D21');

ttr_data_Schmied_650 = xlsread(fn_ttr_data,'Schmid','A2:B12');

```

Figure B.5.: Matlab-script: Load experimental creep data (p.1)

```
%% Transfers the following data:
% ND_Selected_unique:    Number density values of all precipitates exept of
%                        precipitates located in the inner of the subgrains
% MD_Selected_unique:    Mean diameter values of all precipitates exept of
%                        precipitates located in the inner of the subgrains
% ND_unSelected_unique:  Number density values of all precipitates located
%                        in the inner of the subgrains
% MD_unSelected_unique:  Mean diameter values of all precipitates located
%                        in the inner of the subgrains


%% LEGACY CODE Matcalc input from Excel Files

% Open an input dialog window
% prompt = {'name of the Excel file with mean-diameter-data',...
%     'name of the Excel file with number-density-data'};
% dlg_title = 'Excel - Input';
% num_lines = [1 45]; % Size of the input window: height of one letter,
% % width of 45 letters
% default_matcalc_filenames = {'mean_diameter.xlsx','number_density.xlsx'};
% % Suggestion for the names of the Excel files
% matcalc_filenames = inputdlg(prompt,dlg_title,num_lines, ...
% default_matcalc_filenames);


%% Matcalc input from Excel Files

% Numberdensity data
MatCalc_tab_name_ND = ['ND-' MatCalc_tab_name];
% Mean diameter data
MatCalc_tab_name_MD = ['MD-' MatCalc_tab_name];

%% Correction of the arrangement of the columns
% There are some identical columns which contains the same time data.
% Every column, which includes time data, is named "auto"
% Therefore "auto" is used to compare the columns

s1='auto';

% [ND_num, ND_txt, ND_raw] is splitting the table by the following way:
% ND_num: numerical data
% ND_txt: text data
% ND_raw: all data

% The text data is used for the labeling

[ND_num, ND_txt, ND_raw] = xlsread('exp_MatCalc.xlsx',MatCalc_tab_name_ND);
[MD_num, MD_txt, MD_raw] = xlsread('exp_MatCalc.xlsx',MatCalc_tab_name_MD);

% check size to get the correct data for the calculation of the loops
[rows_ND,columns_ND] = size(ND_raw);

% Each first column of the data tabels is the time
% for some easier arrangement the first column is picked up separately
ND_raw_sort = ND_raw(:,1);
MD_raw_sort = MD_raw(:,1);

ND_num_sort = ND_num(:,1);
MD_num_sort = MD_num(:,1);

% In the for loop, the columns of the tables are getting arranged like:
% Time (auto) | Precipitate data 1 |Prec. data 2| Prec. data 3|...

```

Figure B.6.: Matlab-script: Process MatCalc precipitates data (p.1)

process_matcalc_data.m 2 of 4

```
64 for p=1:columns_ND
65     s2=ND_raw(1,p);
66     tf = strcmp(s1,s2);
67 
68     if (tf==0)
69         ND_raw_sort = [ND_raw_sort,ND_raw(:, p)];
70         ND_num_sort = [ND_num_sort,ND_num(:, p)];
71 
72         MD_raw_sort = [MD_raw_sort,MD_raw(:, p)];
73         MD_num_sort = [MD_num_sort,MD_num(:, p)];
74     end
75 end
76 
77 [rows_ND_neu, column_ND_new] = size(ND_raw_sort);
78 
79 % the text data is used to label the GUI
80 Selection_of_Prec_txt = ND_raw_sort(1, 2:column_ND_new);
81 
82 
83 %% Suggestion for the positions of the precipitates
84 % By using the names of the vanadiumnitrides a suggestion for the
85 % positions of the precipitates is generated.
86 % The suggestion is getting inserted in the GUI
87 
88 default_1 = {};
89 VN1 = 'VN(aust,g)';
90 VN2 = 'VN(aust,d)';
91 VN3 = 'VN(aust,s)';
92 VN4 = 'VN(mart,g)';
93 VN5 = 'VN(mart,d)';
94 VN6 = 'VN(mart,s)';
95 
96 for d=1:column_ND_new-1
97 
98     VN = Selection_of_Prec_txt(1,d);
99     tf_VN_1 = strcmp(VN1,VN);
100    tf_VN_2 = strcmp(VN2,VN);
101    tf_VN_3 = strcmp(VN3,VN);
102    tf_VN_4 = strcmp(VN4,VN);
103    tf_VN_5 = strcmp(VN5,VN);
104    tf_VN_6 = strcmp(VN6,VN);
105 
106    if tf_VN_1 || tf_VN_2 || tf_VN_3 || tf_VN_4 || tf_VN_5 || tf_VN_6 == 1
107 
108        default_1 = [default_1, '0'];
109    else
110 
111        default_1 = [default_1, '1'];
112    end
113 
114 end
115 
116 %% - UNCOMMENT IF YOU WANT TO SELECT PRECIPITATE POSITONS
117 %  - (EG NEW MATCALC DATA)
118 
119 %Some explanations of the dialog windows
120 
121 % disp ('In the following window, the precipitates');
122 % disp ('have to be classified according to their positions.');
123 % disp ('A suggestion has already been inserted,');
124 % disp ('however this is to be controlled by the user.');
125 %
126 % disp ('A distiction must be made between precipitates located at');
```

Figure B.7.: Matlab-script: Process MatCalc precipitates data (p.2)

```
127 % disp ('the inner of the subgrains and the outer of the subgrains.');
128 % disp ('Precipitates located at the inner of the subgrains : 0');
129 % disp ('Precipitates located at the outer of the subgrains : 1');
130
131 % correction of the row height because of a to large window
132 %line_hight = 15 / column_ND_new;
133
134 % LEGACY Open an input dialog window for the classification of precipitates
135 % prompt = Selection_of_Prec_txt;
136 % dlg_title = 'Classification of precipitates';
137 % num_lines = [line_hight 45];
138 % matcalc_prec_selection = inputdlg(prompt,dlg_title,num_lines,default_1);
139
140 %%
141
142 matcalc_prec_selection = default_1.'; % .' transponiert matrix
143
144 %% Selection of the positions of the precipitates
145
146 % One table containing the names of the precipitates, located
147 % at the outer of the subgrains, is generated
148 Selection_of_Prec = [Selection_of_Prec_txt.',matcalc_prec_selection]';
149
150 % The starting vector for the data of the precipitates located
151 % at the outer of the subgrains is generated for the number density
152 % and for the mean diameter. Each vector contains the time at the beginning
153 ND_Selected_Prec_num = ND_num_sort(:, 1);
154 MD_Selected_Prec_num = MD_num_sort(:, 1);
155
156 % The starting vector for the data of the precipitates located
157 % at the inner of the subgrains is generated for the number density
158 % and for the mean diameter. Each vector contains the time at the beginning
159
160 ND_unSelected_Prec_num = ND_num_sort(:, 1);
161 MD_unSelected_Prec_num = MD_num_sort(:, 1);
162
163 Selected_Prec_ND = [];
164
165 % In the for loop, the columns of the tables are getting arranged like:
166
167 % Precipitates located at the outer of the subgrains :
168 % Time (auto) | Precipitate data 1 |Prec. data 3| Prec. data 4|...
169
170 % Precipitates located at the inner of the subgrains :
171 % Time (auto) | Precipitate data 2 |Prec. data 5| Prec. data 6|...
172
173 for q=1:column_ND_new-1
174
175     s3='0';
176     s4=Selection_of_Prec(2,q);
177     tf = strcmp(s3,s4);
178
179     if (tf~=1)
180
181     ND_Selected_Prec_num = [ND_Selected_Prec_num,ND_num_sort(:, q+1)];
182     MD_Selected_Prec_num = [MD_Selected_Prec_num,MD_num_sort(:, q+1)];
183     Selected_Prec_ND = [Selected_Prec_ND,Selection_of_Prec(:,q)];
184
185     else
186
187     ND_unSelected_Prec_num = [ND_unSelected_Prec_num,ND_num_sort(:, q+1)];
188     MD_unSelected_Prec_num = [MD_unSelected_Prec_num,MD_num_sort(:, q+1)];
189
```

Figure B.8.: Matlab-script: Process MatCalc precipitates data (p.3)

process_matcalc_data.m 4 of 4

```
190     end
191
192 end
193
194 % If there are some identical time steps, the table is getting corrected
195 % by using the matlab function "unique"
196
197 ND_Selected_unique = unique(ND_Selected_Prec_num,'rows');
198 MD_Selected_unique = unique(MD_Selected_Prec_num,'rows');
199
200 ND_unSelected_unique = unique(ND_unSelected_Prec_num,'rows');
201 MD_unSelected_unique = unique(MD_unSelected_Prec_num,'rows');
202
203 [rows_ND_selected_int,columns_ND_unique] = size(ND_Selected_unique);
204 [rows_ND_unselected_int,columns_ND_unselected_unique] = ...
205     size(ND_unSelected_unique);
206
```

Figure B.9.: Matlab-script: Process MatCalc precipitates data (p.4)

```
%% Excel-files are preloaded in creep-model_start.m


%% Microstructure starting values and parameters

% Starting values of the different dislocation densities
disdens_m = micro_parameters(1,1);
disdens_dip = micro_parameters(2,1);
disdens_b = micro_parameters(3,1);

% Total dislocation density [m^-2]
disdens_t = micro_parameters(4,1);

% Subgrain radius [m]
R_sbg = micro_parameters(6,1);

% M23C6 (T)
rp1 = micro_parameters(9,1); % mean radius [m]
rp01 = micro_parameters(9,1); % initial radius [m]
Nvp01 = micro_parameters(10,1); % number density [m^-3]

% MX (martensite) (T)
rp2 = micro_parameters(13,1); % mean radius [m]
rp02 = micro_parameters(13,1); % initial radius [m]
Nvp02 = micro_parameters(14,1); % number density [m^-3]

% MX (austenite) (T)
rp3 = micro_parameters(17,1); % mean radius [m]
rp03 = micro_parameters(17,1); % initial radius [m]
Nvp03 = micro_parameters(18,1); % number density [m^-3]

% Shear modulus [Pa] (T)
% in Ghoniem called μ
G = micro_parameters(20,1);

% Burgers vector [m]
b = micro_parameters(21,1);
% one lattice parameter

% Activation-energy for dislocations [J]
Q = micro_parameters(22,1);

% Atomic Volume [m^3]
omega = micro_parameters(23,1);
% from PhD-Thesis Fritz Krumphals - spheric volume with half atomic
% distance as radius


%% Model starting values and parameters

% damageparameter A
A = mod_parameters(1,1);

% Damageparameter a1
a1 = mod_parameters(2,1);

%
rate_0 = mod_parameters(3,1);

% Size of the unit cell [m]
ag = mod_parameters(4,1);

% Taylorfactor: Relation of the shear flow stress of a single crystal to
```

Figure B.10.: Matlab-script: Process parameter excel file (p.1)

parameters.m 2 of 2

```
64 % the uniaxial flow stress of a polycrystal
65 M = mod_parameters(6,1);
66
67 % alpha: dislocation interaction constant from Abe?
68 alpha = mod_parameters(7,1);
69
70 % annihilation length danh
71 d_anh = mod_parameters(8,1);
72
73 % Weight factor for dislocation stress field
74 c_dip = mod_parameters(9,1);
75
76 % Coarsening parameter for M23C6
77 Kd1 = mod_parameters(12,1);
78 Kp1 = mod_parameters(13,1);
79
80 % Coarsening parameter for MX
81 Kd2 = mod_parameters(16,1);
82 Kp2 = mod_parameters(17,1);
83
84 % Activation energy for Pipediffusion
85 W = mod_parameters(19,1);
86
87 % Transfer coefficient of vacancies from the dislocation core to jogs
88 eta = mod_parameters(20,1);
89
90 % Constant that accounts for the fraction of dipoles that annihilate when
91 % transforming to boundary dislocations (for eq.(6) in Yadav)
92 zeta = mod_parameters(21,1);
93
94 % Spacing of dislocation boundary [m]
95 Hd = mod_parameters(22,1);
96
97 % Poisson's ratio
98 ny = mod_parameters(23,1);
99
100 % self diffusion coefficient
101 Ds = mod_parameters(24,1);
102
103 % pipe diffusion coefficient
104 Dvp = mod_parameters(25,1);
105
106 % Beta
107 beta = mod_parameters(27,1);
108
109 % Constant climb velocity
110 vc_neu = mod_parameters(28,1);
111
```

Figure B.11.: Matlab-script: Process parameter excel file (p.2)

```
%% Function for Matcalc data
% Transfers the following data:
% ND_Selected_unique:    Number density values of all precipitates exept of
%                        the precipitates located in the inner of the
%                        subgrains
% MD_Selected_unique:    Mean diameter values of all precipitates exept of
%                        the precipitates located in the inner of the
%                        subgrains
% ND_unSelected_unique:  Number density values of all precipitates located
%                        in the inner of the subgrains
% MD_unSelected_unique:  Mean diameter values of all precipitates located
%                        in the inner of the subgrains

%% LEGACY CODE
% if matcalc == 1
%     [ND_Selected_unique,MD_Selected_unique, ND_unSelected_unique,...
%         MD_unSelected_unique] = processing_matcalc_data();
%
%     [rows_ND_selected_int,columns_ND_unique] = size(ND_Selected_unique);
%     [rows_ND_unselected_int,columns_ND_unselected_unique] =...
%         size(ND_unSelected_unique);
% end

%% Generating an empty matrix for time to rupture diagram data
% if there is none existing because of missing earlier calculations

if exist('time_to_rupture_diagram_matrix','var') == 1
else
    time_to_rupture_diagram_matrix = [];
end

%% create and update progress bar
loop_counter = loop_counter+1;
waitbar((loop_counter/(sigma_applied_steps+1)),f,...
    ['calculating creep curve nr. ' num2str(loop_counter) ' of ' ...
    num2str(sigma_applied_steps) ' ...'],'Name',script_version);

%% Starting conditions

TIME_STEP = 10^(-5);
v_eff = 0;
Msb = 0;
time = 0;
strain = 0;
rate_Rsb = 0;
rate_b=0;
rate_m=0;

% Damage Parameters
D_cav=0;
D_prc1=0;
D_prc2=0;
D_prc=0;

% Convert from MPa to Pa
sigma_applied_current = sigma_applied_stepper*10^6;

% Generating an empty table for saving all the simulation data
data = zeros(NUMBER_OF_ITERATIONS,24);

%% Main loop

for i=1:NUMBER_OF_ITERATIONS
```

Figure B.12.: Matlab-script: Main model file with all calculations (p.1)

main_model.m 2 of 7

```
64
65 %Corrected applied strain (STRESS??) with lateral strain
66 sigma_applied = sigma_applied_current*(1+strain*0.3);
67
68 % Internal stress (eq. (3) in Yadav)
69 sigma_i = alpha*G*M*b*sqrt(c_dip*disdens_dip+disdens_m);
70
71 % Effective stress (eq. (2) in Yadav)
72 sigma_effective = sigma_applied - sigma_i;
73
74 % LEGACY CODE
75 % Glide velocity (eq.(1) in Yadav or eq. (12) in Ghoniem)
76 % vg = a1*exp((-Q)/(k*T))*sigma_effective*(omega/(k*T));
77
78 % a2 = 16.55; LEGACY
79 omega_mult=21.8; % FIXME Where to put this number
80 vg = a1*exp((-Q)/(k*T))*exp(-sigma_i*omega*omega_mult/(k*T))...
81     *2*sinh(sigma_applied*omega*omega_mult/(k*T));
82 % TODO: CHECK if input is correct (sinh in Matlab is in RADIANS)
83
84 % Path length for diffussion along the core
85 % (eq.(15_125) in Theory of dislocations)
86 Lp = ag*sqrt(2)*exp(W/(2*k*T));
87
88 % Climb velocity for pipe diffusion (eq. (34) in Ghoniem)
89 vcp = (2*pi*b*Dvp*sigma_effective*omega)/(Lp^2*k*T);
90
91 % Length that is governing the range of the elastic interaction between
92 % the dislocation and the defects (eq. (20) in Ghoniem)
93 L_alpha_v = ((1+ny)*G*b*0.5*omega)/(3*pi*(1-ny)*k*T);
94
95 % Climb velocity for lattice diffusion (eq. (27)+(26)+(24) in Ghoniem)
96 vcl = ((2*pi*eta*Ds*omega*sigma_effective)/...
97     ((1-(eta*log(L_alpha_v*sqrt(disdens_t))))*b*k*T));
98
99 % Summed climb velocity of dislocations (Ghoniem)
100 vc =(vcp+vcl);
101
102 % Surface energy of the subgrain boundary (eq. (36) in Ghoniem)
103 Ysb = (G*b^2*disdens_b*R_sbg)/3;
104
105 % Subgrain-growth pressure (eq. (38) in Ghoniem)
106 Ps = (4*G*b^2*disdens_b)/3;
107
108 % Dislocation spacing within the subgrain walls (eq.(3) in Ghoniem)
109 Hb = 1/((disdens_b+disdens_dip)*R_sbg);
110
111
112 %% Saving the simulation data every time step
113
114 data(i,1)  = time;
115 data(i,2)  = strain;
116 data(i,3)  = disdens_m;
117 data(i,4)  = disdens_dip;
118 data(i,5)  = disdens_b;
119 data(i,6)  = disdens_t;
120 data(i,7)  = R_sbg;
121 data(i,8)  = sigma_applied;
122 data(i,9)  = rp1;
123 data(i,10) = rp2;
124 data(i,11) = sigma_effective;
125 data(i,12) = sigma_i;
126 data(i,13) = vg;
```

Figure B.13.: Matlab-script: Main model file with all calculations (p.2)

```
127 data(i,14) = vc;
128 data(i,15) = Ysb;
129 data(i,16) = Ps;
130 data(i,17) = Hb;
131 data(i,18) = Msb;
132 data(i,19) = D_cav;
133 data(i,20) = D_prc1;
134 data(i,21) = D_prc2;
135 data(i,22) = D_prc;
136 data(i,23) = v_eff;
137 data(i,24) = vc_neu;
138
139 %% Calculation of the number density without MatCalc data
140 Nvp1 = Nvp01*rp01^3/rp1^3;
141 Nvp2 = Nvp02*rp02^3/rp2^3;
142
143 %% Calculation with MatCalc data
144 % Because of the variable time step, an interpolation of the MatCalc data
145 % is necessary. For that interpolation the matlab function interp1 is
146 % used.
147
148 if matcalc_choice == 1
149
150 % for example the data of table "ND_Selected_unique" is getting
151 % interpolated by using the function interp1 by using the first
152 % column (time), where the function is looking for the correct row
153 % (time / 3600 because of hours to seconds) and is interpolating
154 % the correct value in a linear way.
155
156     ND_selected_int=interp1(ND_Selected_unique(:,1),...
157         ND_Selected_unique,time/3600,'linear');
158     MD_selected_int=interp1(MD_Selected_unique(:,1)...
159         ,MD_Selected_unique,time/3600,'linear');
160
161     ND_unselected_int=interp1(ND_unSelected_unique(:,1)...
162         ,ND_unSelected_unique,time/3600,'linear');
163     MD_unselected_int=interp1(MD_unSelected_unique(:,1)...
164         ,MD_unSelected_unique,time/3600,'linear');
165
166     %starting values for the following loop
167
168     rN_selected = 0;
169     rN_eff_unselected = 0;
170     Nvp_eff_unselected = 0;
171
172     % loop for the calculation of the sum of Nvp_i*rp_i^2
173     % of the precipitates located in subgrains and subgrain boundarys
174     for m=2:columns_ND_unique
175         rN_selected = rN_selected + ND_selected_int(1,m)*...
176             (MD_selected_int(1,m)/(2*10^9))^2;
177     end
178
179
180     % loop for the calculation of the effective radius and numberdenity
181     % of the precipitates located in dislocations
182     for n=2:columns_ND_unselected_unique
183         rN_eff_unselected = rN_eff_unselected + ND_unselected_int(1,n)*...
184             (MD_unselected_int(1,n)/(2*10^9));
185         Nvp_eff_unselected = Nvp_eff_unselected + ND_unselected_int(1,n);
186     end
187
188     r_eff_unselected = rN_eff_unselected / Nvp_eff_unselected;
189
```

Figure B.14.: Matlab-script: Main model file with all calculations (p.3)

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```
190     % constraint for mobility of subgrains (eq.(41) in Ghoniem)
191     if Ps > 2*pi*(rN_selected)*Ysb
192         % mobility of subgrains (eq.(39)+(40) in Ghoniem)
193         Msb = ((2*pi*eta*Ds*omega)/(b*k*T))+...
194         ((2*pi*b*Dvp*omega)/(Hb^2*k*T));
195     end
196
197     % constraint for mobility of subgrains (eq.(41) in Ghoniem)
198     if Ps < 2*pi*(rN_selected)*Ysb
199         % mobility of subgrains (eq.(43) in Ghoniem)
200         Msb = Ds*omega/(4*pi*(rp1^4+rp2^4)*(Nvp1+Nvp2)*k*T);
201     end
202
203     % boundary dislocation rate (eq.(6) in Yadav)
204     rate_b = ((8-zeta)*disdens_dip*vc_neu/Hb)- ...
205     (disdens_b*Msb/R_sbg*...
206     (Ps-(2*pi*rN_selected*Ysb)));
207
208     % subgrain grow rate (eq.(7) in Yadav)
209     rate_Rsb = Msb*(Ps-(2*pi*(rN_selected)*Ysb));
210
211     % effective velocity of mobile dislocations due to a
212     % consideration of Prof. Sonderegger.
213     v_eff = vg*vc/(vc+vg*(Nvp_eff_unselected*r_eff_unselected^3)*pi/2);
214 end
215
216 %% Calculation without MatCalc data
217
218 if matcalc_choice == 0
219     % Constraint for mobility of subgrains (eq.(41) in Ghoniem)
220     if Ps > 2*pi*(rp1^2*Nvp1+rp2^2*Nvp2)*Ysb
221
222         % mobility of subgrains (eq.(39)+(40) in Ghoniem)
223         Msb = ((2*pi*eta*Ds*omega)/(b*k*T))+...
224         ((2*pi*b*Dvp*omega)/(Hb^2*k*T));
225
226     end
227
228     % constraint for mobility of subgrains (eq.(41) in Ghoniem)
229     if Ps < 2*pi*(rp1^2*Nvp1+rp2^2*Nvp2)*Ysb
230
231         % Mobility of subgrains (eq.(43) in Ghoniem)
232         Msb = Ds*omega/(4*pi*(rp1^4+rp2^4)*(Nvp1+Nvp2)*k*T);
233
234     end
235
236     % Boundary dislocation rate (eq.(6) in Yadav)
237     rate_b = ((8-zeta)*disdens_dip*vc_neu/Hb)- ...
238     (disdens_b*Msb/R_sbg*...
239     (Ps-(2*pi*(rp1^2*Nvp1+rp2^2*Nvp2)*Ysb)));
240
241     % Subrain grow rate (eq.(7) in Yadav)
242     rate_Rsb = Msb*(Ps-(2*pi*(rp1^2*Nvp1+rp2^2*Nvp2)*Ysb));
243
244     % Calculation of v_eff is not possible without MatCalc data
245     v_eff = 0;
246 end
247
248
249 %% Calculation without v_eff
250
251 if v_eff_choice == 0
252
```

Figure B.15.: Matlab-script: Main model file with all calculations (p.4)

```
253     % Mobile dislocation rate (eq.(4) in Yadav)
254     rate_m = (vg*disdens_m^(3/2)-(vg*disdens_m/(2*R_sbg))-...
255     (8*disdens_m^(3/2)*vc_neu)+beta*vg*R_sbg/(Hb^2)-...
256     (d_anh*disdens_m*(disdens_m+disdens_dip)*vg));
257
258     % Dipole dislocation rate (eq.(5) in Yadav)
259     rate_dip = (vg*disdens_m/(2*R_sbg))-(8*disdens_dip*vc_neu/Hb)-...
260     (d_anh*disdens_m*disdens_dip*vg);
261
262 end
263
264 %% Calculation with v_eff
265
266 if v_eff_choice == 1
267
268     % Mobile dislocation rate (eq.(4) in Yadav)
269     rate_m = (v_eff*disdens_m^(3/2)-(v_eff*disdens_m/(2*R_sbg))-...
270     (8*disdens_m^(3/2)*vc_neu)+beta*v_eff*R_sbg/(Hb^2)-...
271     (d_anh*disdens_m*(disdens_m+disdens_dip)*v_eff));
272
273     % Dipole dislocation rate (eq.(5) in Yadav)
274     rate_dip = (v_eff*disdens_m/(2*R_sbg))-(8*disdens_dip*vc_neu/Hb)-...
275     (d_anh*disdens_m*disdens_dip*v_eff);
276
277 end
278
279 %% Calculation with the modified Orowan equation
280
281 if damage_choice == 1
282
283     if v_eff_choice == 0
284     rate_strain = disdens_m*vg*b/((1-D_prc)*(1-D_cav)*M);
285     end
286
287     if v_eff_choice == 1
288     rate_strain = disdens_m*v_eff*b/((1-D_prc)*(1-D_cav)*M);
289     end
290
291 end
292
293 %% Calculation with the Orowan equation
294
295 if damage_choice == 0
296
297     if v_eff_choice == 0
298     rate_strain = disdens_m*vg*b/M;
299     end
300
301     if v_eff_choice == 1
302     rate_strain = disdens_m*v_eff*b/M;
303     end
304
305 end
306
307 %% Precipitate coarsening
308 % Note: No precipitation coarsening of rp3
309
310 rp1 = (Kd1*data(i,1)+rp01^3)^(1/3);
311 l_MC = 4; % for M23C6 (can also be set outside of loop)
312
313 rp2 = (Kd2*data(i,1)+rp02^3)^(1/3);
314 l_MX = 6; % for MX (can also be set outside of loop)
315
```

Figure B.16.: Matlab-script: Main model file with all calculations (p.5)

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```
316
317
318 %% Calculation of the damage parameter
319
320 % Coarsening of Precipitates (eq.(10)+(11) in Yadav)
321 D_prc1 = 1-(Kp1*data(i,1)+1)^(1/(1-l_MC));
322 D_prc2 = 1-(Kp2*data(i,1)+1)^(1/(1-l_MX));
323 D_prc = 1-((1-D_prc1)^(-1)*(1-D_prc2)^(-1))^(-1);
324
325 % Caviation softening (eq.(12) in Yadav)
326 rate_D_cav = (A*rate_strain*strain);
327
328 %% Calculation of the variable time step
329
330 Timestep_m = abs((percentage_change*disdens_m)/(100*rate_m));
331 Timestep_dip = abs((percentage_change*disdens_dip)/(100*rate_dip));
332 Timestep_b = abs((percentage_change*disdens_b)/(100*rate_b));
333 Timestep_Rsb = abs((percentage_change*R_sbg)/(100*rate_Rsb));
334 Timestep_strain = abs((percentage_change*strain)/(100*rate_strain));
335 Timestep_Dcav = abs((percentage_change*D_cav)/(100*rate_D_cav));
336
337 % Chosing the smallest step
338 TIME_STEP = min([Timestep_m Timestep_dip Timestep_b Timestep_Rsb ...
339     Timestep_strain Timestep_Dcav]);
340
341 if TIME_STEP == 0
342     TIME_STEP = 10^(-5);
343 end
344
345 %% Timestep
346 time = time + TIME_STEP;
347
348 %% Calculation after timestep
349
350 disdens_m = disdens_m + rate_m*TIME_STEP;
351 disdens_dip = disdens_dip + rate_dip*TIME_STEP;
352 disdens_b = (disdens_b + rate_b*TIME_STEP);
353 disdens_t = disdens_m + disdens_dip + disdens_b;
354 R_sbg = R_sbg + rate_Rsb*TIME_STEP;
355 D_cav = D_cav + rate_D_cav*TIME_STEP;
356 strain = strain + rate_strain*TIME_STEP;
357
358 %% Break options
359
360 if disdens_m < 0
361     disp('Error : disdens_m < 0');
362     return
363 end
364
365 if disdens_dip < 0
366     disp('Error : disdens_dip < 0');
367     return
368 end
369
370 if disdens_b < 0
371     disp('Error : disdens_b < 0');
372     return
373 end
374
375 if time >= (1.5 * TIME_MAX * 3600) %TODO find good/better value or solution
376     data = data(1:i,:);
377     break
378 end
```

Figure B.17.: Matlab-script: Main model file with all calculations (p.6)

```
379
380 if D_cav >= 1 || D_prc >= 1
381     data = data(1:i,:);
382     break
383 end
384
385 if damage_choice == 1
386     if strain >= 0.06
387         data = data(2:i,:);
388         break
389     end
390 end
391
392 if damage_choice == 0
393     if strain >= 0.025
394         data = data(2:i,:);
395         break
396     end
397 end
398
399 end
400
401 %% prepare data for diagrams and figures
402 data(:,1) = data(:,1)/3600; % convert time from [s] to [h]
403 data(:,2) = data(:,2)*100; % convert strain from [] to [%]
404 rup_time_mod = time/3600;
405
406 %% counter and divider for stress level loop
407 sigma_applied_figure = sigma_applied_stepper;
408 sigma_applied_stepper = (sigma_applied_stepper - (sigma_applied_start ...
409     - sigma_applied_end) / (sigma_applied_steps - 1) );
410
```

Figure B.18.: Matlab-script: Main model file with all calculations (p.7)

plot_figures.m 1 of 1

```
%% Prepare additional title

if matcalc_choice == 1
   matcalc_title = 'with MatCalc data';
else
   matcalc_title = 'fast calculation';
end

%% Plot the simulated data

figure('Name',creep_tab_name,'NumberTitle','off')
plot(data(:,1),data(:,2),'-k')
hold on
plot(CreepData(:,1),CreepData(:,2),'--k')
title(['Creep curve at ' num2str(sigma_applied_current/1000000) ...
    ' MPa - (' num2str(matcalc_title) ')'])
xlabel('time [h]'); ylabel('strain [%]')
legend('calculated',['experimental data: ' num2str(creep_tab_name)],...
    'location','northeast')

%% preserve data for time to rupture diagram

time_to_rupture_diagram_data = [sigma_applied_current time/3600];
time_to_rupture_diagram_matrix = [time_to_rupture_diagram_matrix;...
    time_to_rupture_diagram_data];


%% LEGACY CODE: preserve data for time to rupture diagram

% After a successful creep simulation the following question appears.
% answer_save_data = questdlg(...
% 'Save data for the calculation of a time to rupture diagram?',...
% 'time to rupture diagram', 'Yes', 'No', 'Yes');
%
% switch answer_save_data
%     case 'Yes'
%     disp('saved')
%     time_to_rupture_diagram_choice = 1;
%
%     case 'No'
%     time_to_rupture_diagram_choice = 2;
% end

% By pressing the "yes" button the data of the stress and time is saved
% to a table with some data from some past calculations

% if time_to_rupture_diagram_choice == 1
%     time_to_rupture_diagram_data = [sigma_applied_current time/3600];
%     time_to_rupture_diagram_matrix = [time_to_rupture_diagram_matrix;...
%     time_to_rupture_diagram_data];
% end

```

Figure B.19.: Matlab-script: Plot experimental and simulated creep curve (p.1)

```
%% Update waitbar progress
waitbar(1,f,'Finishing diagrams ...','Name',script_version);
close(f)

%% LEGACY CODE Plot creep data

% After the saving the following question appears.
% answer_plot_rupture_diagram = ...
%    questdlg('Do you want to plot the time to rupture diagram?',...
% 'time to rupture diagram', 'Yes', 'No', 'Yes');
%
% switch answer_plot_rupture_diagram
%     case 'Yes'
%     time_to_rupture_diagram_choice = 1;
%     case 'No'
%     time_to_rupture_diagram_choice = 2;
% end

% By pressing the "yes" button the time to rupture diagram is getting
% plotted.

% if time_to_rupture_diagram_choice == 1

%% Generate time to rupture (TTR) diagram

time_to_rupture_diagram_matrix = ...
    unique(time_to_rupture_diagram_matrix,'rows');
time_to_rupture_diagram_matrix = ...
    sortrows(time_to_rupture_diagram_matrix,1);

% Generating the calculated time to rupture figure
figure
loglog(time_to_rupture_diagram_matrix(:,2),...
    time_to_rupture_diagram_matrix(:,1)/1e6,'-pr','LineWidth',2);
title(['time to rupture (for given T) - (' num2str(matcalc_title) ')'])
xlabel('time [h]'); ylabel('stress [MPa]')

grid on
hold on

% plot experimental data
loglog(ttr_data_ECCC(:,1),ttr_data_ECCC(:,2),'-.^','color',[1 0.5 0],...
    'MarkerIndices',1:5:length(ttr_data_ECCC(:,2)));
loglog(ttr_data_ASME(:,1),ttr_data_ASME(:,2),'-.v','color',[1 0.5 0]);

loglog(ttr_data_NIMS_650_MgA(:,1),ttr_data_NIMS_650_MgA(:,2),...
    '-.*','color',[1 0.5 0]);
loglog(ttr_data_NIMS_650_MgB(:,1),ttr_data_NIMS_650_MgB(:,2),...
    '-.+','color',[1 0.5 0]);
loglog(ttr_data_NIMS_650_MgC(:,1),ttr_data_NIMS_650_MgC(:,2),...
    '-.o','color',[1 0.5 0]);

loglog(ttr_data_NIMS_600_MgA(:,1),ttr_data_NIMS_600_MgA(:,2),...
    '-.*','color',[0.1 0.4 0.2]);
loglog(ttr_data_NIMS_600_MgB(:,1),ttr_data_NIMS_600_MgB(:,2),...
    '-.+','color',[0.1 0.4 0.2]);
loglog(ttr_data_NIMS_600_MgC(:,1),ttr_data_NIMS_600_MgC(:,2),....
    '-.o','color',[0.1 0.4 0.2]);

loglog(ttr_data_NIMS_550_MgA(:,1),ttr_data_NIMS_550_MgA(:,2),....
    '-.*','color',[0.1 0.2 0.8]);
loglog(ttr_data_NIMS_550_MgB(:,1),ttr_data_NIMS_550_MgB(:,2),....
    '-.+','color',[0.1 0.2 0.8]);
```

Figure B.20.: Matlab-script: Plot time to rupture diagram (p.1)

time_to_rupture_diagram.m 2 of 2

```
64 loglog(ttr_data_NIMS_550_MgC(:,1),ttr_data_NIMS_550_MgC(:,2),....
65     '-.o','color',[0.1 0.2 0.8]);
66
67 loglog(ttr_data_Hxx_625(:,1),ttr_data_Hxx_625(:,2),'-.*m');
68 loglog(ttr_data_Hxx_600(:,1),ttr_data_Hxx_600(:,2),'-.+m');
69 loglog(ttr_data_Hxx_575(:,1),ttr_data_Hxx_575(:,2),'-.om');
70
71 loglog(ttr_data_Schmied_650(:,1),ttr_data_Schmied_650(:,2),'-.pb');
72
73 legend([num2str(T-273.15) '°C - calculated'],...
74     '650°C - BM - ECCC','650°C - BM - ASME',...
75     '650°C - NIMS - MgA','650°C - NIMS - MgB','650°C - NIMS - MgC',...
76     '600°C - NIMS - MgA','600°C - NIMS - MgB','600°C - NIMS - MgC',...
77     '550°C - NIMS - MgA','550°C - NIMS - MgB','550°C - NIMS - MgC',...
78     '625°C - P91 weld','600°C - P91 weld','575°C - P91 weld',...
79     '650°C - Schmid 2018','location','southwest')
80
81 hold off
82
```

Figure B.21.: Matlab-script: Plot time to rupture diagram (p.2)

Appendix C.

Detailed MatCalc precipitation kinetics results

	phase fraction [%]			mean diameter [nm]			number density [m^{-3}]		
service at 550°C	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h
M23C6 (mart,sgb)	2,262	2,262	2,262	119	149	271	2,36E+19	1,09E+19	1,86E+18
Laves (mart,sgb)	0,539	0,552	0,556	29,9	58,5	95,5	3,35E+20	4,60E+19	1,06E+19
Laves (mart,di)	0,163	0,160	0,161	30,5	59,1	97,9	9,49E+19	1,24E+19	2,82E+18
VN (aust,gb)	0,012	0,017	0,014	246	676	1130	1,50E+16	8,98E+14	1,46E+14
VN (aust,sgb)	0,276	0,275	0,289	23,3	28,4	41,3	3,49E+20	1,96E+20	7,14E+19
VN (mart,gb)	0,119	0,114	0,102	169	268	417	4,52E+17	1,04E+17	2,58E+16
NbC (aust,gb)	0,001	0,001	0,001	107	107	105	1,63E+16	1,63E+16	1,63E+16
NbC (mart,gb)	0,031	0,031	0,031	52,3	61,5	106	3,90E+18	2,24E+18	4,71E+17
mod. Z (aust,gb)	0,000	0,000	0,000	217	217	217	2,09E+13	2,09E+13	2,09E+13
mod. Z (mart,gb)	0,000	0,000	0,000	68,3	68,7	70,8	1,15E+15	1,15E+15	1,15E+15

Table C.1.: 550°C service: phase properties

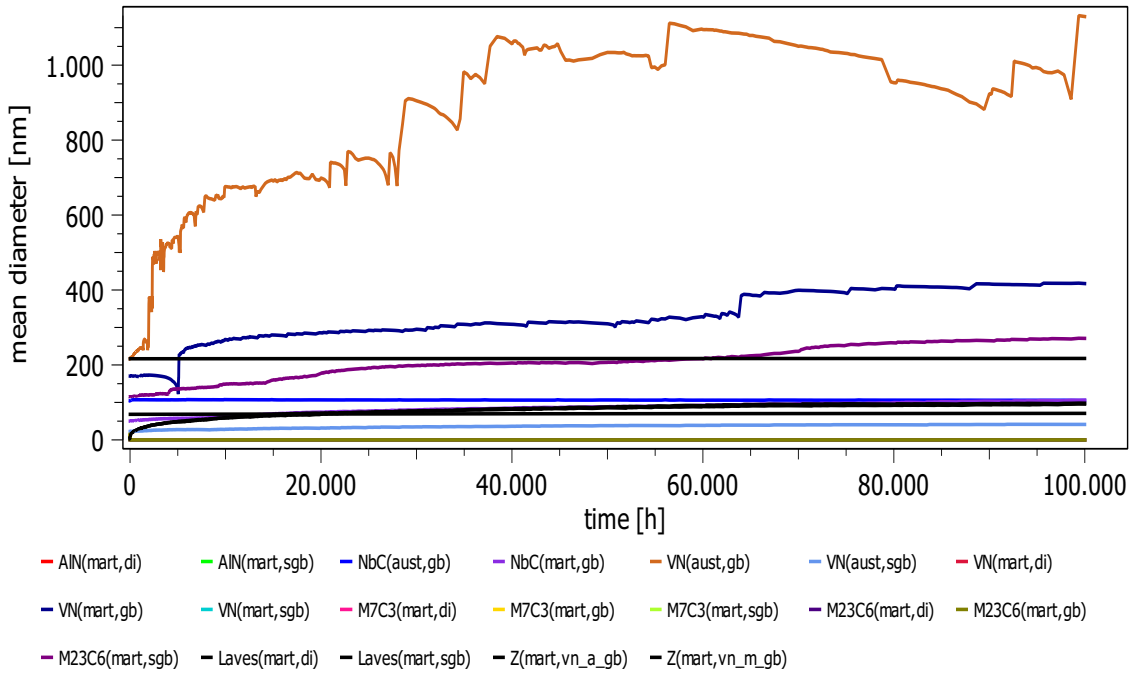

Figure C.1.: 550°C service: mean diameter diagram

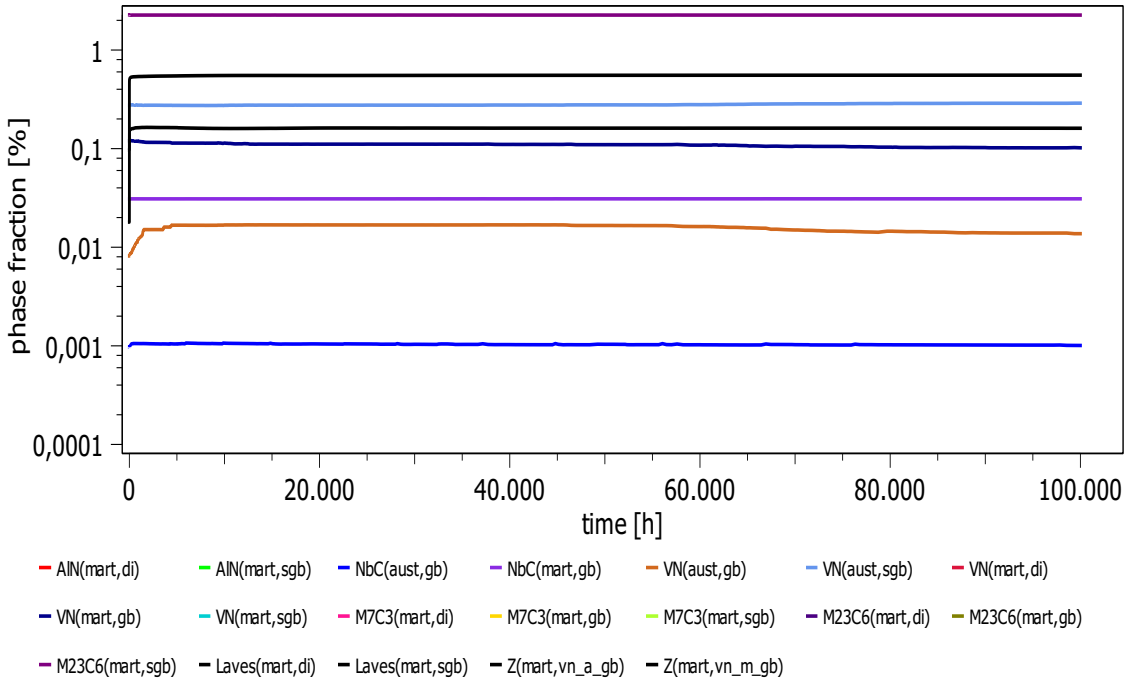

Figure C.2.: 550°C service: phase fraction diagram

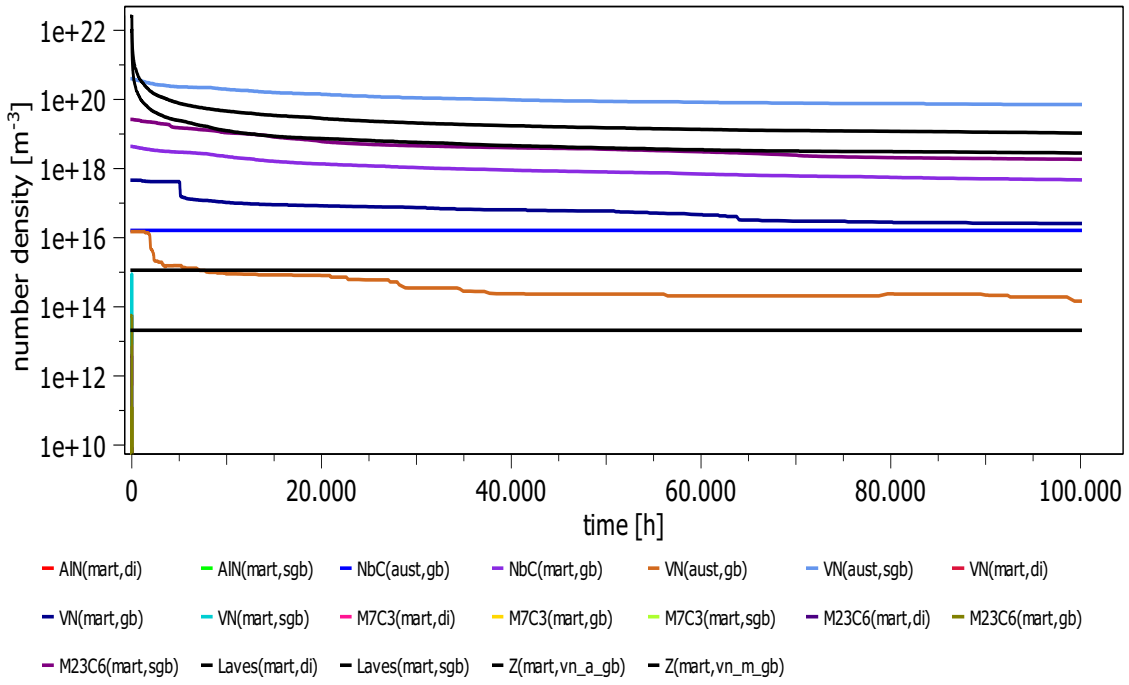

Figure C.3.: 550°C service: number density diagram

	phase fraction [%]			mean diameter [nm]			number density [m^{-3}]		
service at 575°C	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h
M23C6 (mart,sgb)	2,262	2,262	2,262	122	205	357	2,05E+19	4,04E+18	8,26E+17
Laves (mart,sgb)	0,491	0,498	0,509	41,6	83,8	148	1,10E+20	1,44E+19	2,58E+18
Laves (mart,di)	0,105	0,108	0,104	41,6	84,3	135	2,39E+19	3,04E+18	6,82E+17
VN (aust,gb)	0,010	0,011	0,015	630	645	694	7,33E+14	7,71E+14	7,74E+14
VN (aust,sgb)	0,274	0,280	0,311	25,0	34,9	51,8	2,89E+20	1,09E+20	3,73E+19
VN (mart,gb)	0,118	0,112	0,078	174	287	416	4,23E+17	8,14E+16	1,83E+16
NbC (aust,gb)	0,001	0,001	0,001	106	106	108	1,63E+16	1,63E+16	1,36E+16
NbC (mart,gb)	0,031	0,031	0,031	55,0	78,8	132	3,35E+18	1,13E+18	2,40E+17
mod. Z (aust,gb)	0,000	0,000	0,000	217	217	219	2,09E+13	2,09E+13	2,09E+13
mod. Z (mart,gb)	0,000	0,000	0,000	68,4	69,7	99,7	1,15E+15	1,15E+15	1,15E+15

Table C.2.: 575°C service: phase properties

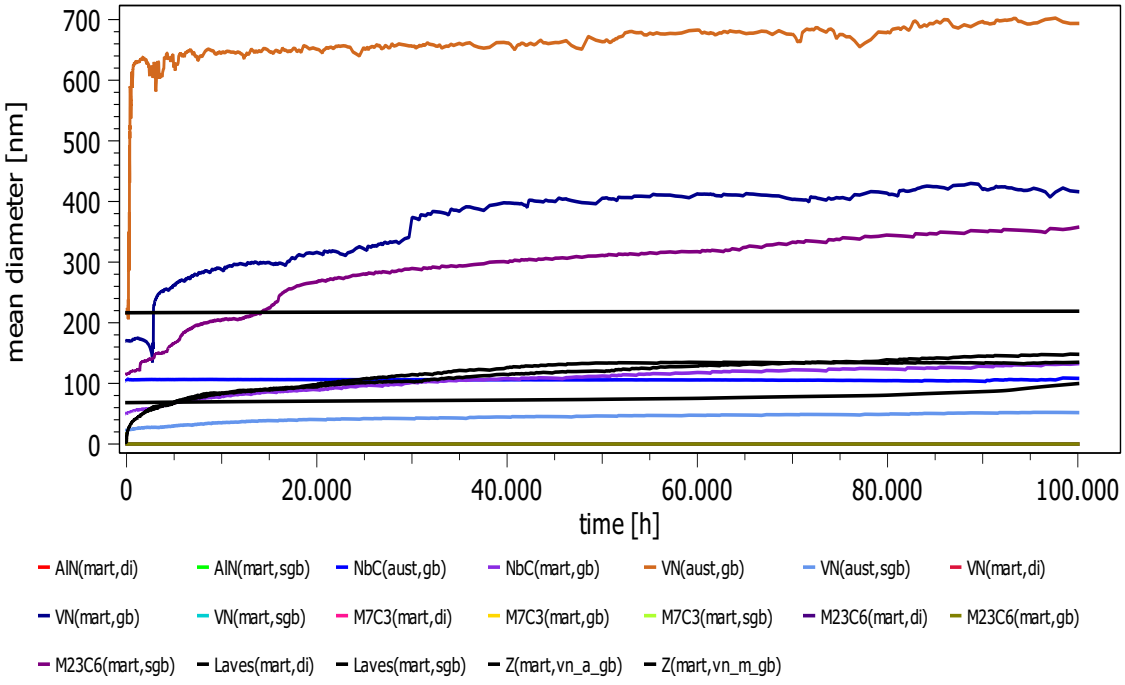

Figure C.4.: 575°C service: mean diameter diagram

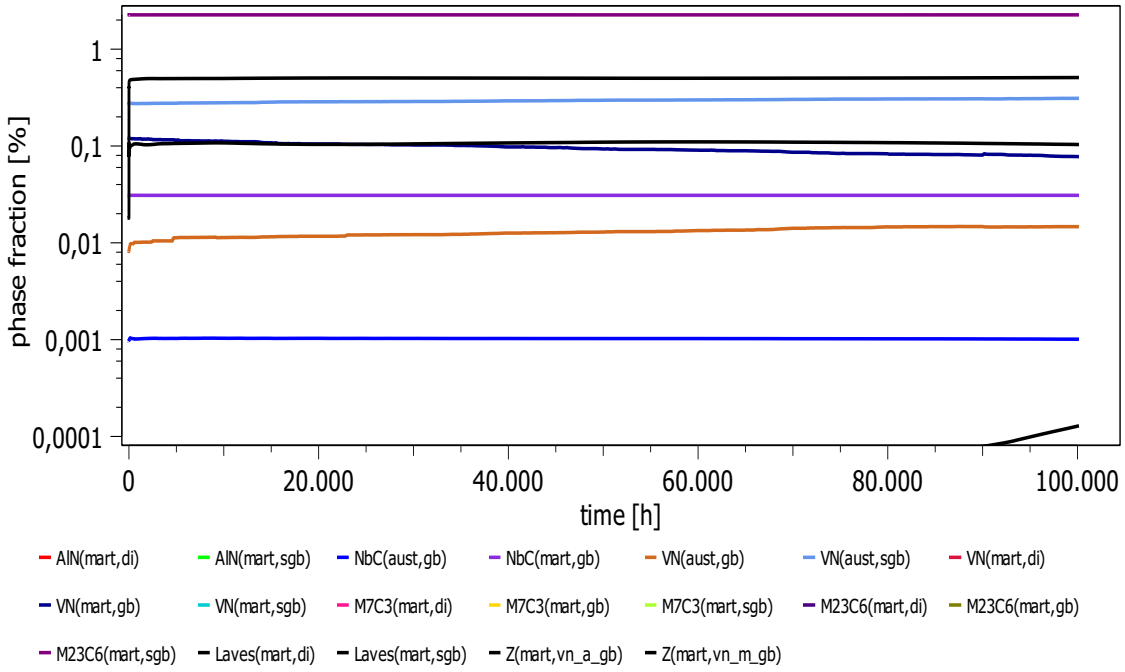

Figure C.5.: 575°C service: phase fraction diagram

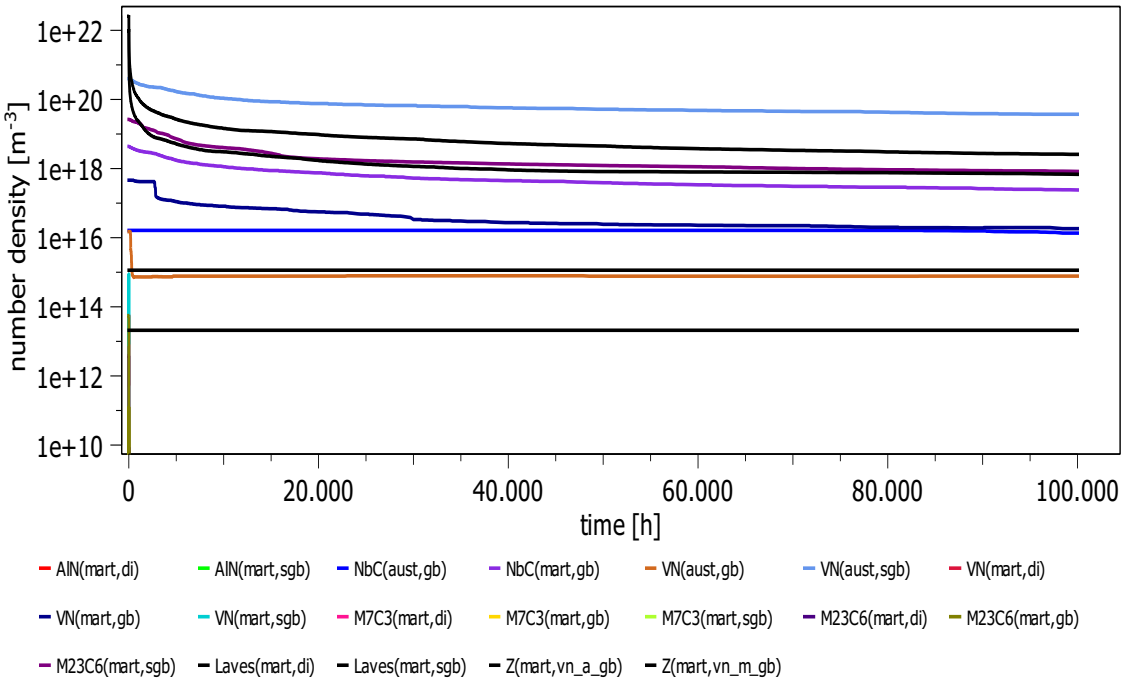

Figure C.6.: 575°C service: number density diagram

	phase fraction [%]			mean diameter [nm]			number density [m^{-3}]		
service at 600°C	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h
M23C6 (mart,sgb)	2,262	2,262	2,262	142	298	468	1,22E+19	1,41E+18	3,84E+17
Laves (mart,sgb)	0,387	0,386	0,411	57,7	120	205	3,31E+19	3,47E+18	7,86E+17
Laves (mart,di)	0,067	0,079	0,062	60,3	121	211	4,91E+18	7,68E+17	1,15E+17
VN (aust,gb)	0,009	0,029	0,026	259	729	699	5,84E+15	1,33E+15	1,31E+15
VN (aust,sgb)	0,273	0,290	0,368	27,1	43,0	74,5	2,31E+20	6,25E+19	1,44E+19
VN (mart,gb)	0,119	0,083	0,001	167	346	703	4,20E+17	3,34E+16	4,91E+13
NbC (aust,gb)	0,001	0,001	0,001	106	107	158	1,63E+16	1,63E+16	3,36E+15
NbC (mart,gb)	0,031	0,031	0,031	58,5	96,7	162	2,76E+18	6,06E+17	1,29E+17
mod. Z (aust,gb)	0,000	0,000	0,000	217	218	222	2,09E+13	2,09E+13	2,09E+13
mod. Z (mart,gb)	0,000	0,000	0,011	68,7	71,7	569	1,15E+15	1,15E+15	1,15E+15

Table C.3.: 600°C service: phase properties

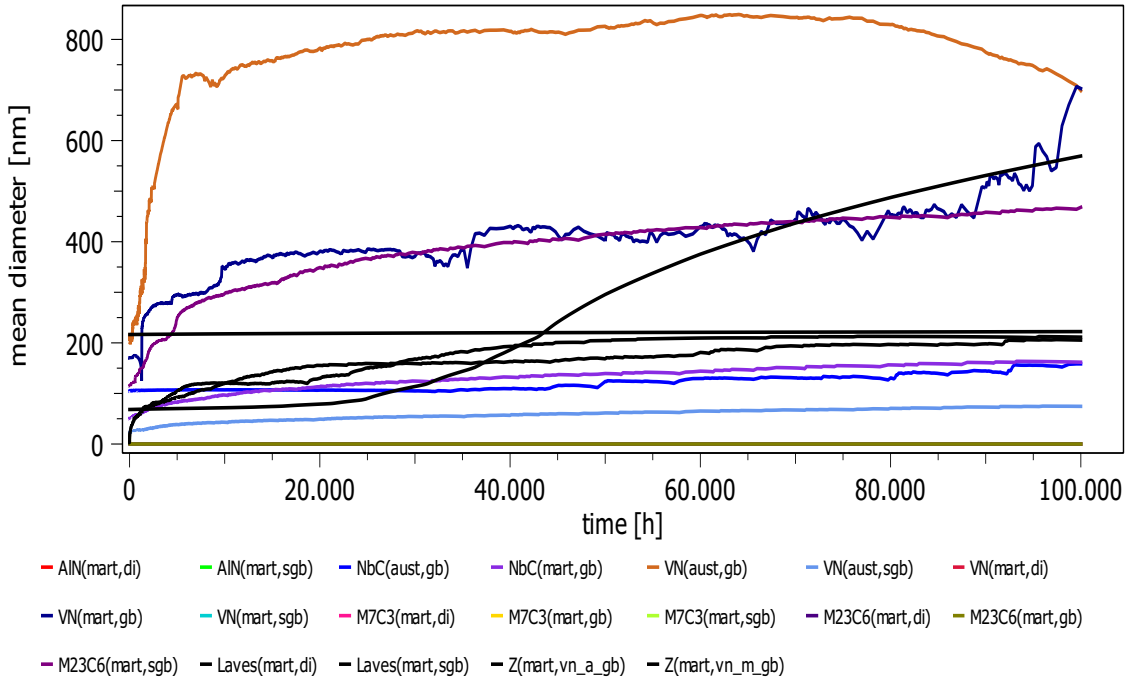

Figure C.7.: 600°C service: mean diameter diagram

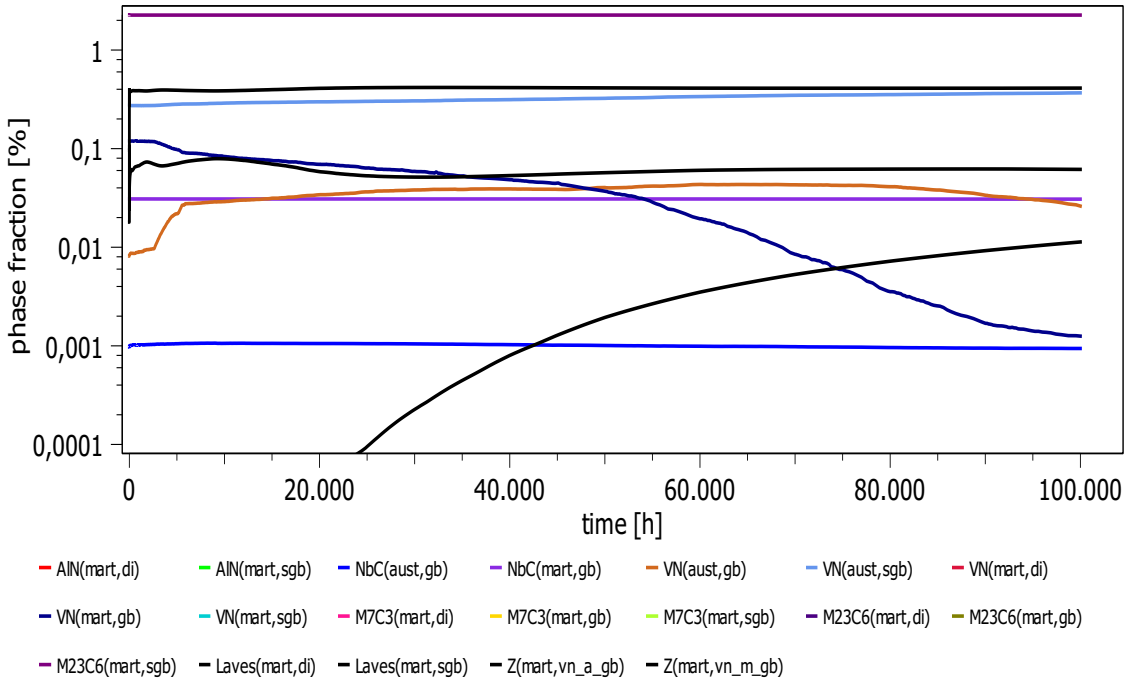

Figure C.8.: 600°C service: phase fraction diagram

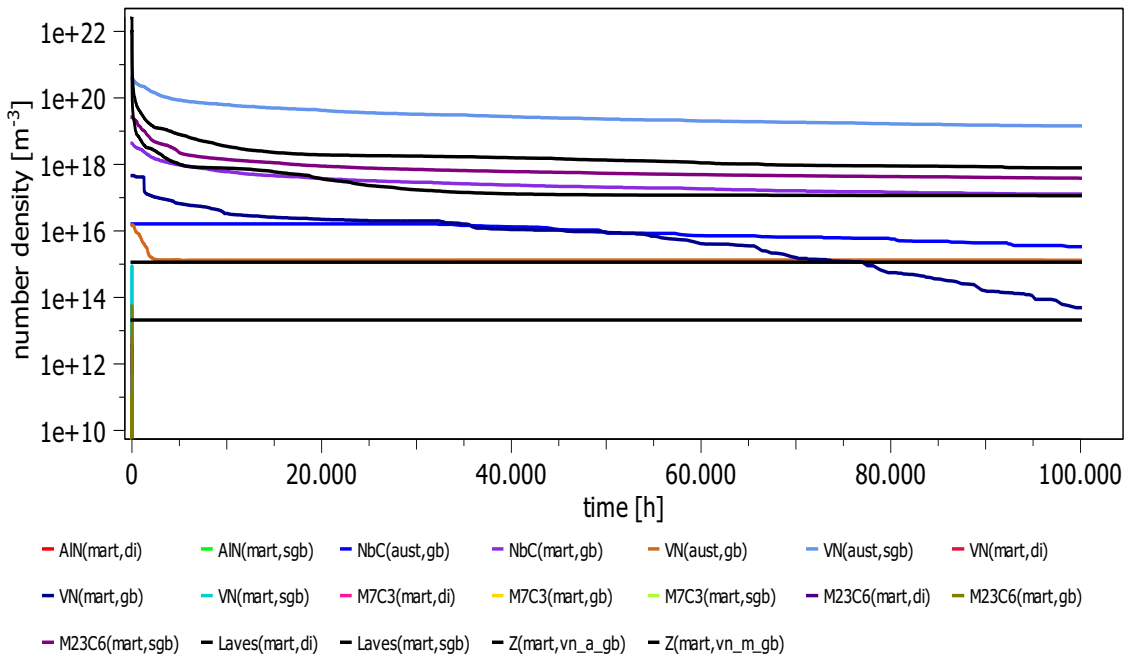

Figure C.9.: 600°C service: number density diagram

	phase fraction [%]			mean diameter [nm]			number density [m^{-3}]		
service at 625°C	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h
M23C6 (mart,sgb)	2,261	2,261	2,265	199	388	611	4,52E+18	6,54E+17	1,70E+17
Laves (mart,sgb)	0,207	0,237	0,271	79,1	172	316	6,50E+18	7,62E+17	1,51E+17
Laves (mart,di)	0,061	0,042	0,016	81,7	185	307	1,68E+18	1,20E+17	9,65E+15
VN (aust,gb)	0,008	0,010	0,001	307	545	526	2,93E+15	1,18E+15	1,64E+14
VN (aust,sgb)	0,272	0,272	0,282	31,9	53,3	98,3	1,35E+20	2,91E+19	5,09E+18
VN (mart,gb)	0,120	0,117	0,070	269	455	586	1,08E+17	2,17E+16	5,07E+15
NbC (aust,gb)	0,001	0,001	0,001	107	106	276	1,63E+16	1,63E+16	8,28E+14
NbC (mart,gb)	0,031	0,031	0,029	72,9	120	202	1,43E+18	3,23E+17	6,42E+16
mod. Z (aust,gb)	0,000	0,000	0,000	217	220	356	2,09E+13	2,09E+13	2,09E+13
mod. Z (mart,gb)	0,000	0,000	0,072	69,3	146	1061	1,15E+15	1,15E+15	1,15E+15

Table C.4.: 625°C service: phase properties

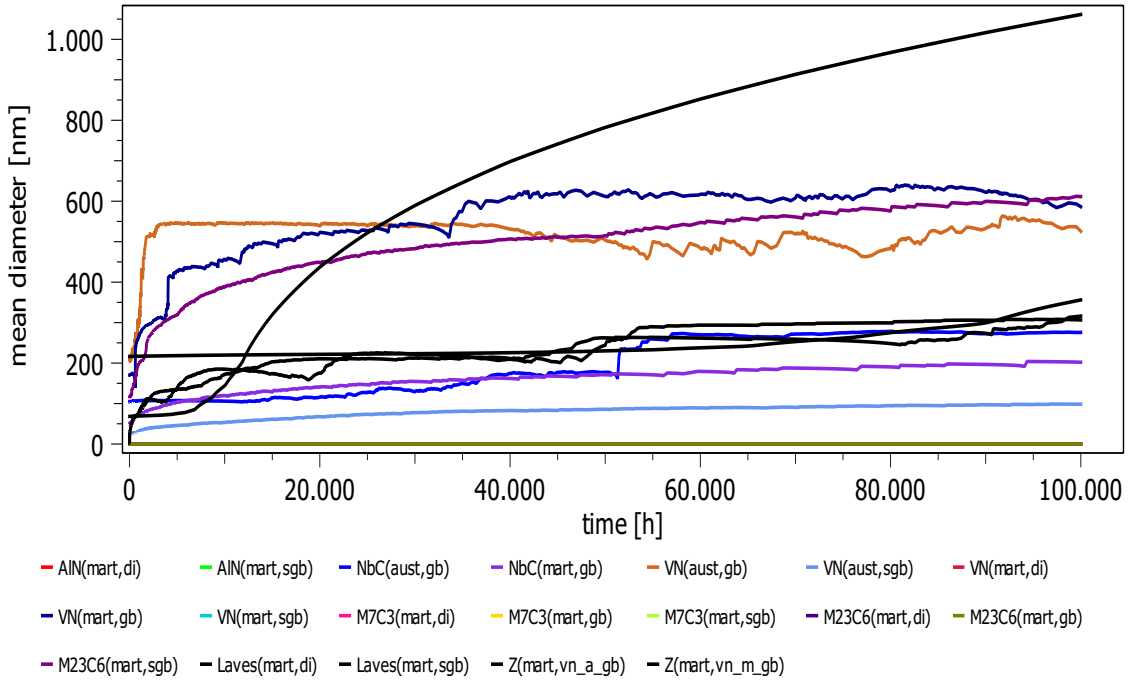

Figure C.10.: 625°C service: mean diameter diagram

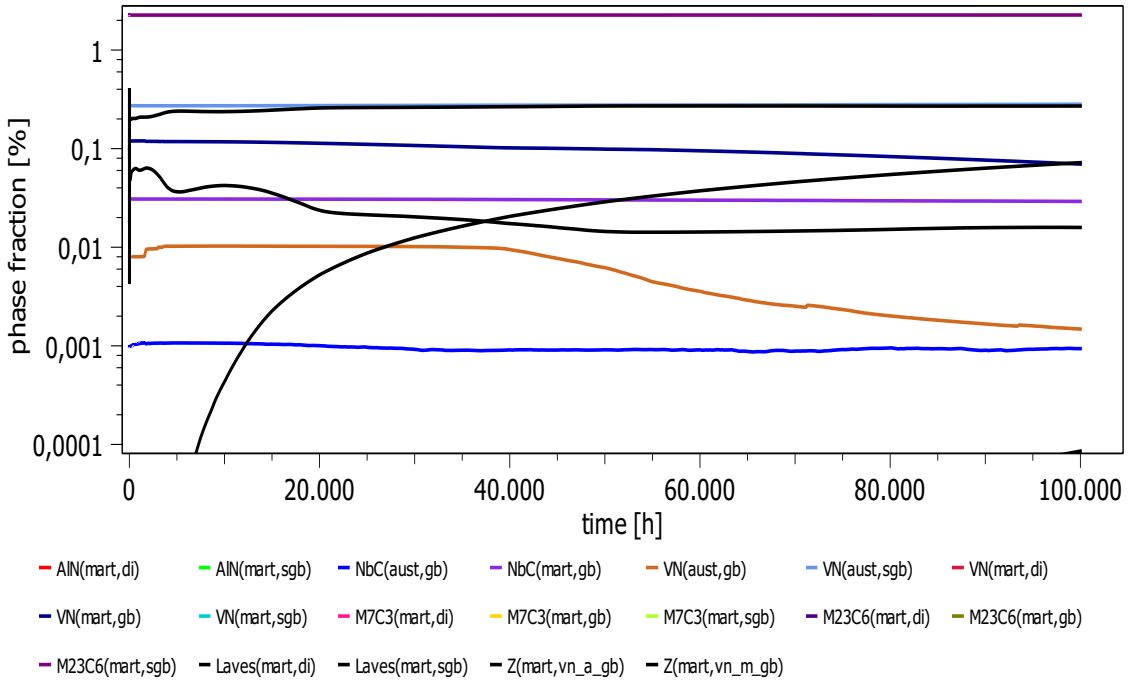

Figure C.11.: 625°C service: phase fraction diagram

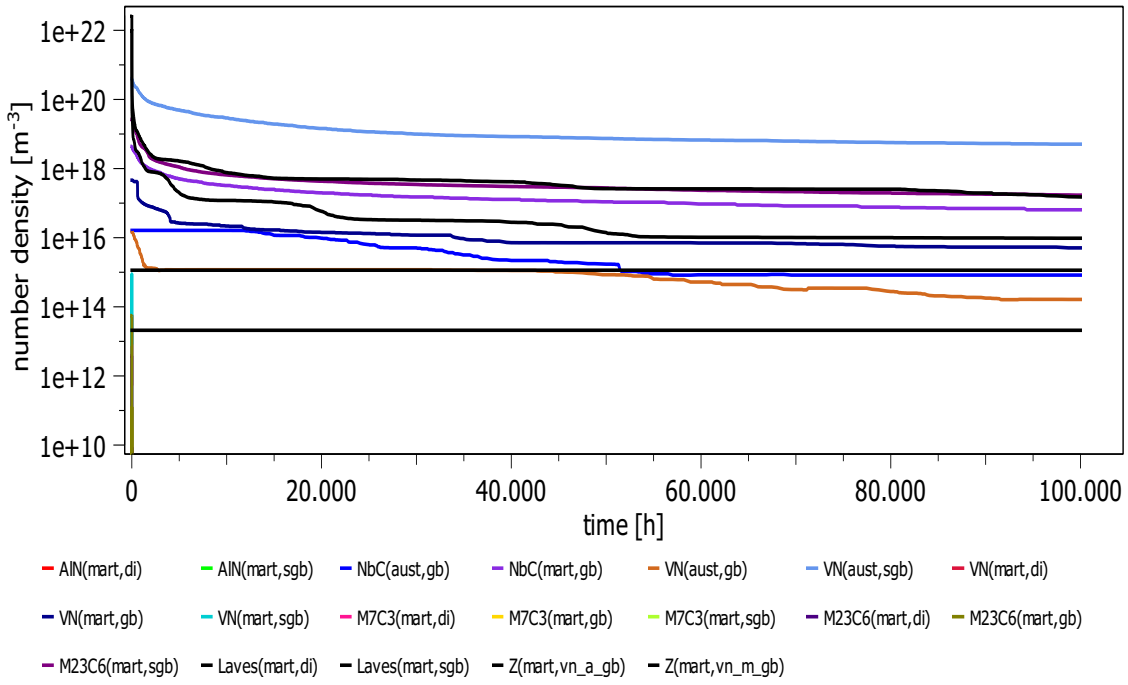

Figure C.12.: 625°C service: number density diagram

	phase fraction [%]			mean diameter [nm]			number density [m^{-3}]		
service at 650°C	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h	1000 h	10 000 h	100 000 h
M23C6 (mart,sgb)	2,260	2,262	2,286	283	496	816	1,64E+18	3,24E+17	7,22E+16
Laves (mart,sgb)	0,000	0,000	0,000	0,00	0,00	0,00	0,00E+00	0,00E+00	0,00E+00
Laves (mart,di)	0,000	0,000	0,000	0,00	0,00	0,00	0,00E+00	0,00E+00	0,00E+00
VN (aust,gb)	0,019	0,019	0,000	544	551	0,00	2,14E+15	2,14E+15	0,00E+00
VN (aust,sgb)	0,269	0,273	0,160	40,4	80,1	119	7,14E+19	9,19E+18	1,60E+18
VN (mart,gb)	0,110	0,095	0,000	292	696	0,00	7,61E+16	4,89E+15	0,00E+00
NbC (aust,gb)	0,001	0,001	0,000	108	202	0,00	1,63E+16	2,57E+15	0,00E+00
NbC (mart,gb)	0,031	0,030	0,021	87,7	151	236	8,23E+17	1,58E+17	2,89E+16
mod. Z (aust,gb)	0,000	0,000	0,002	218	223	1307	2,09E+13	2,09E+13	2,09E+13
mod. Z (mart,gb)	0,000	0,019	0,361	75,4	620	1658	1,49E+15	1,49E+15	1,49E+15

Table C.5.: 650°C service: phase properties

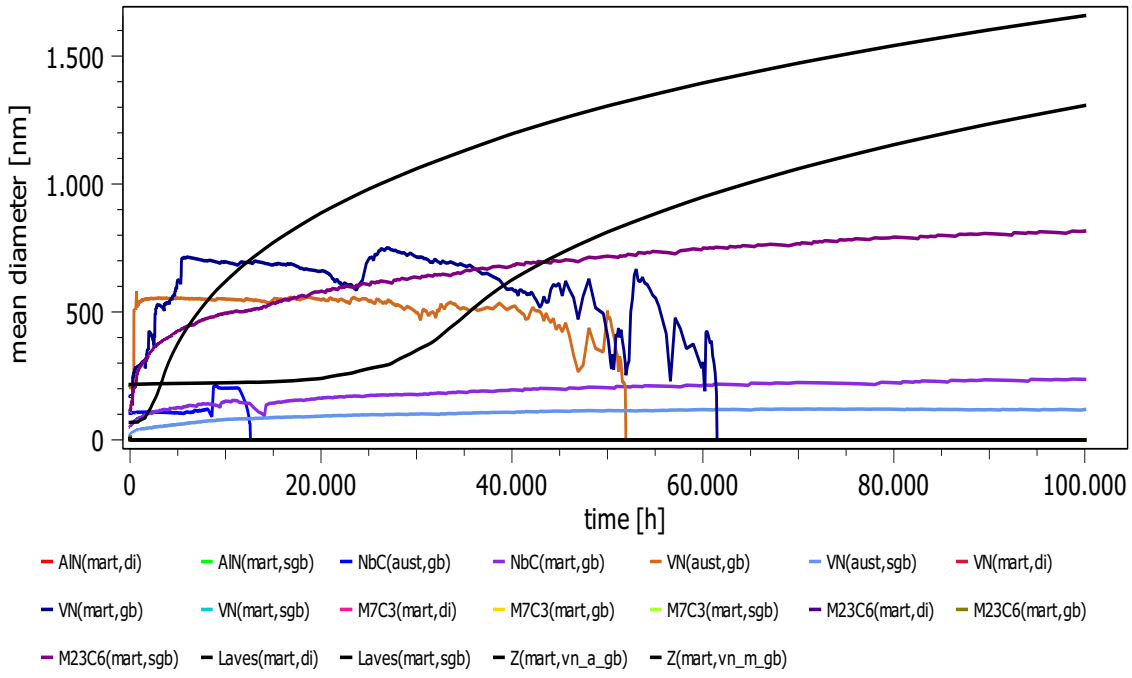

Figure C.13.: 650°C service: mean diameter diagram

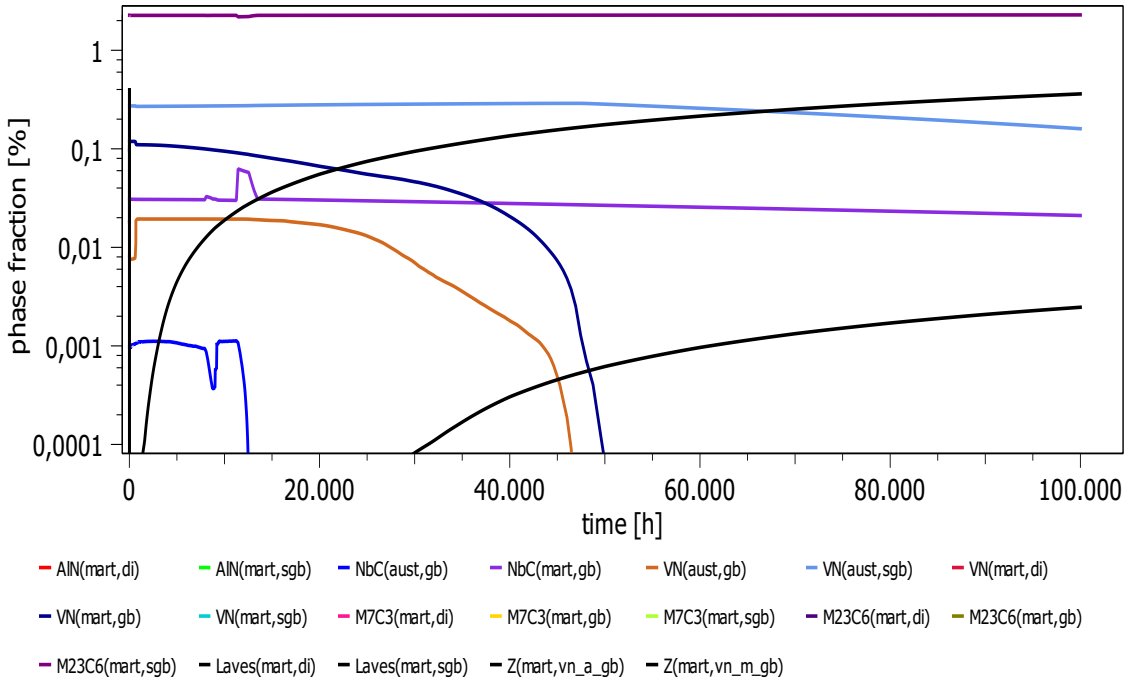

Figure C.14.: 650°C service: phase fraction diagram

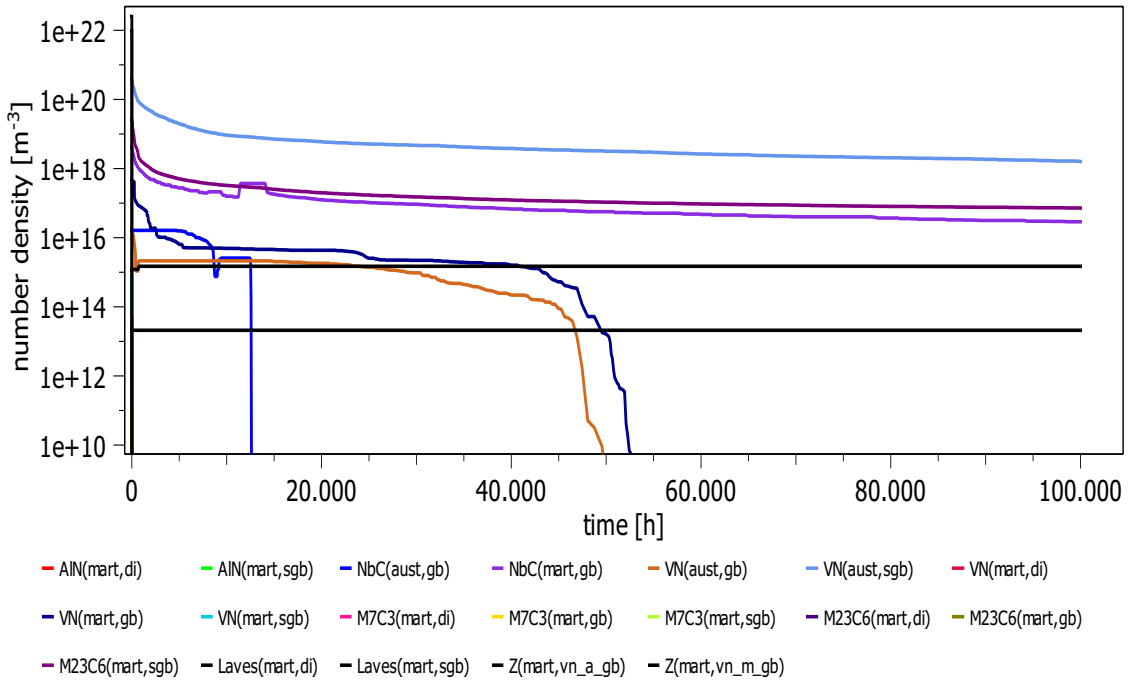

Figure C.15.: 650°C service: number density diagram

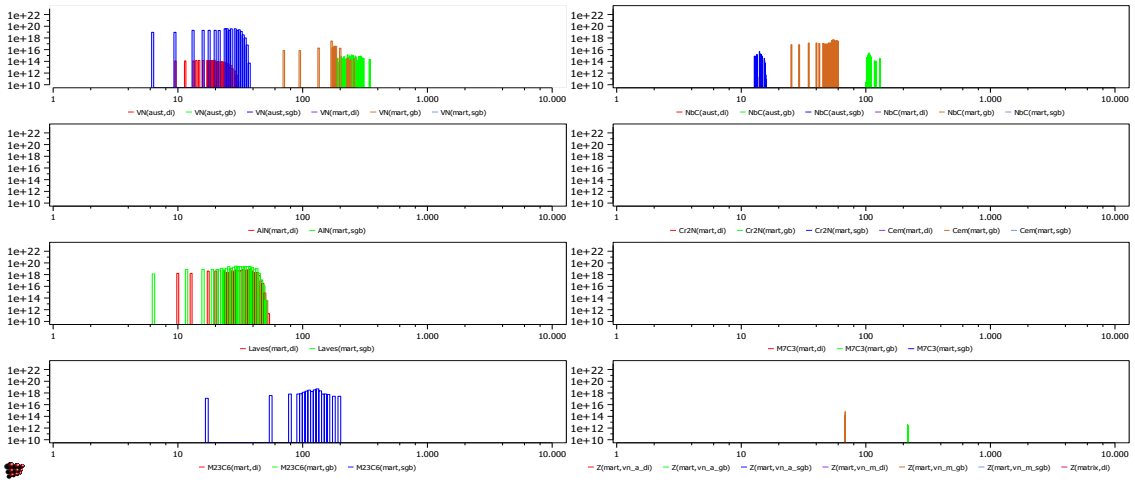

Figure C.16.: 550°C service: precipitate size classes distribution after 1 000 h

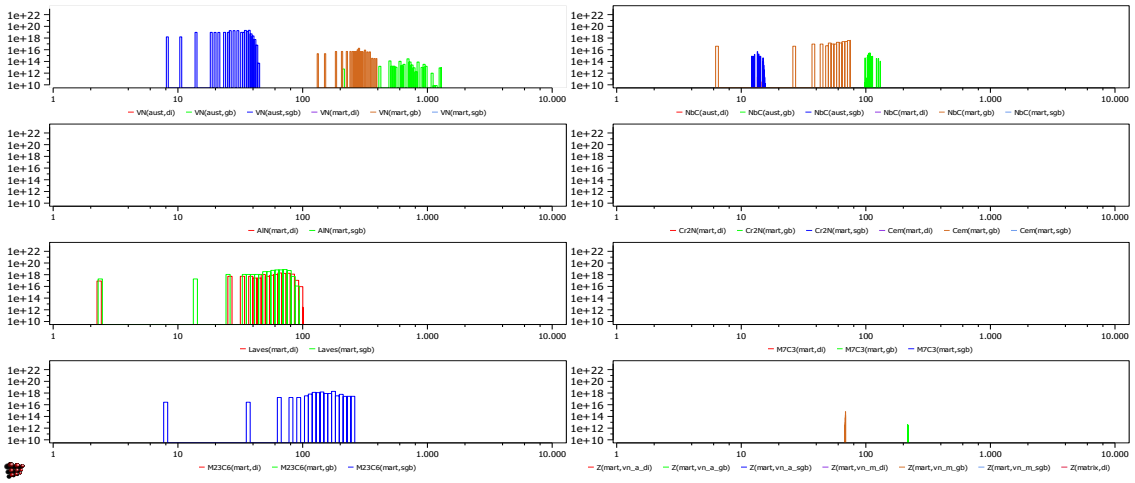

Figure C.17.: 550°C service: precipitate size classes distribution after 10 000 h

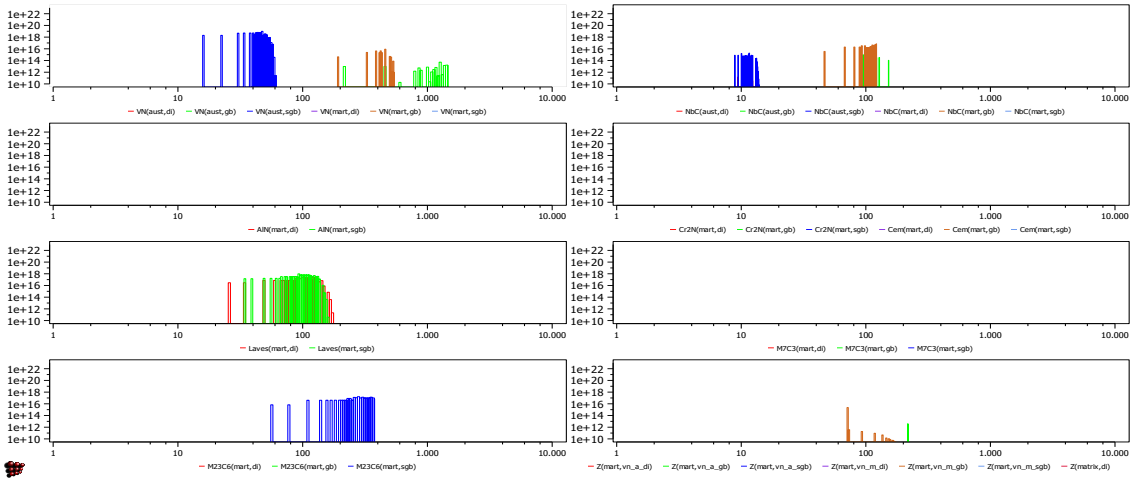

Figure C.18.: 550°C service: precipitate size classes distribution after 100 000 h

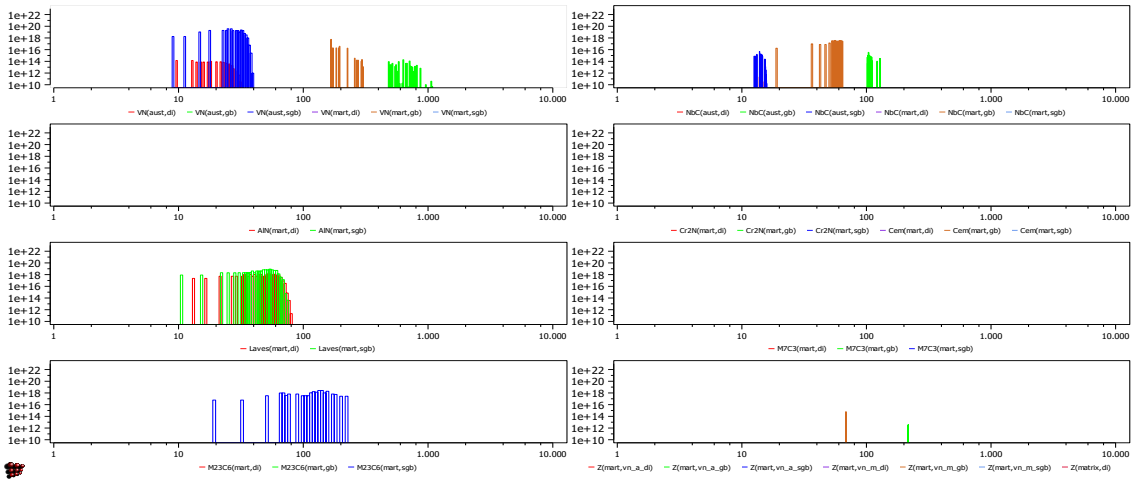

Figure C.19.: 575°C service: precipitate size classes distribution after 1 000 h

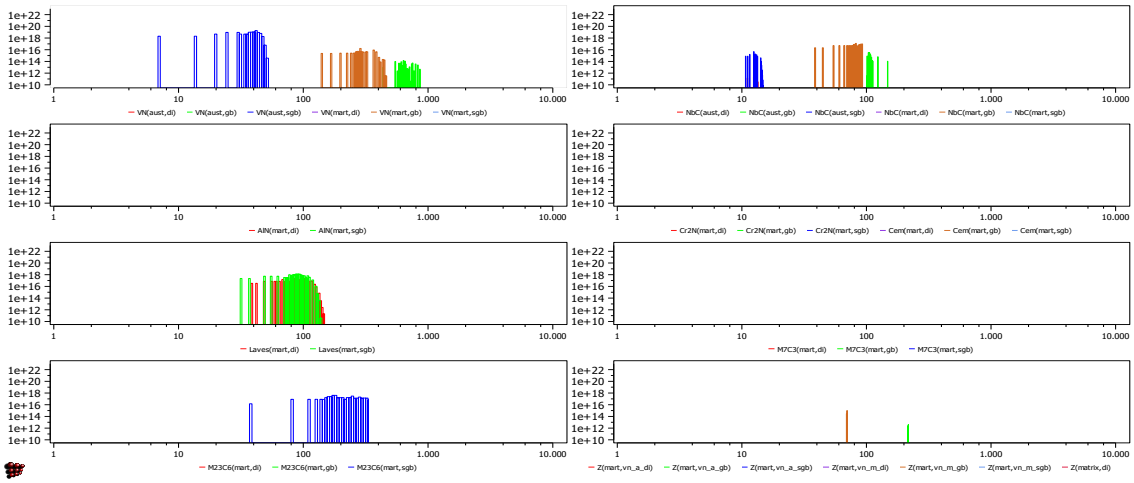

Figure C.20.: 575°C service: precipitate size classes distribution after 10 000 h

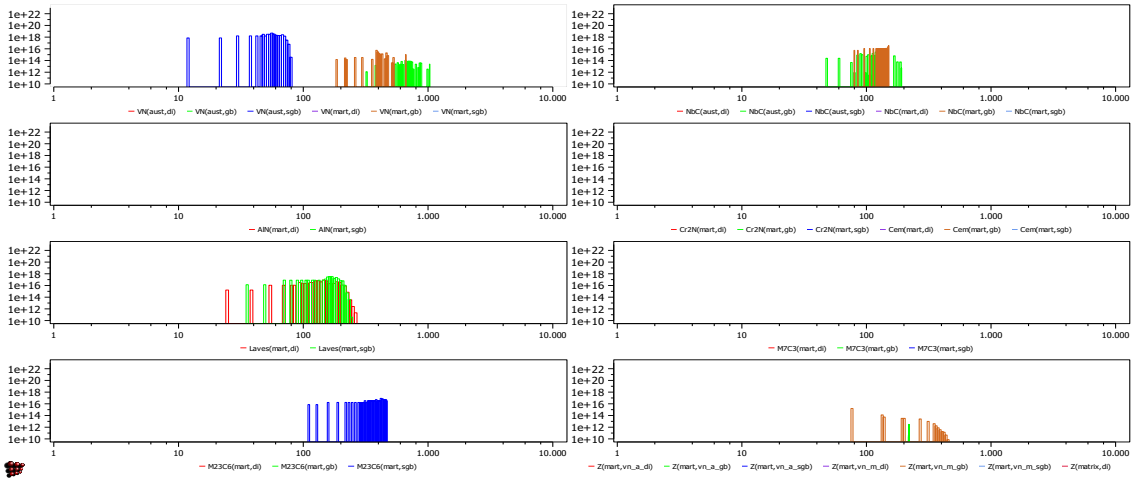

Figure C.21.: 575°C service: precipitate size classes distribution after 100 000 h

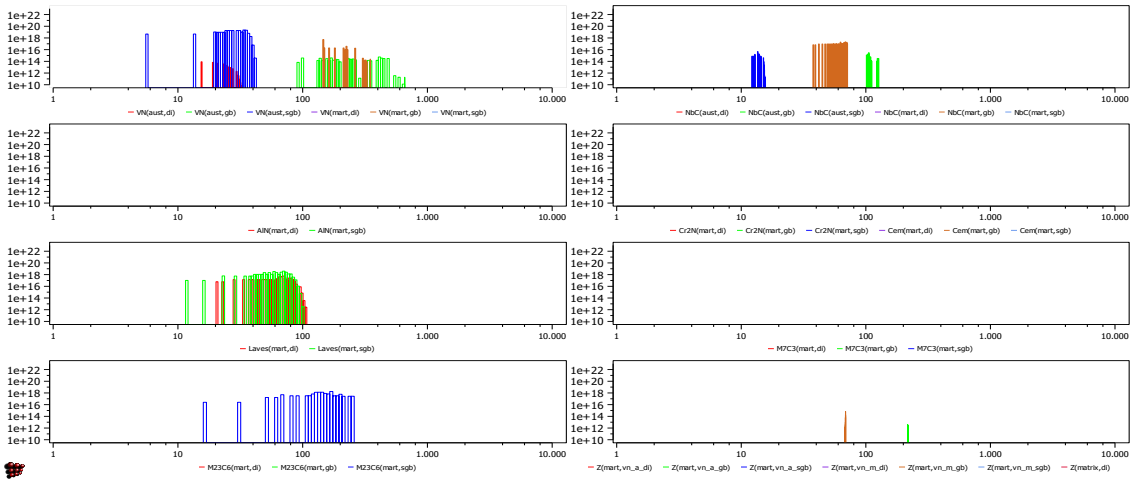

Figure C.22.: 600°C service: precipitate size classes distribution after 1 000 h

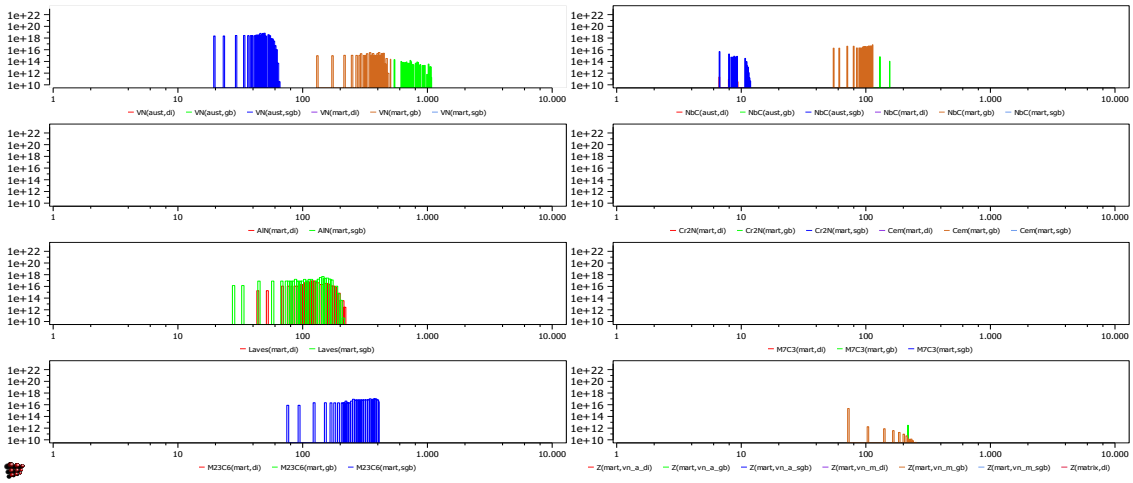

Figure C.23.: 600°C service: precipitate size classes distribution after 10 000 h

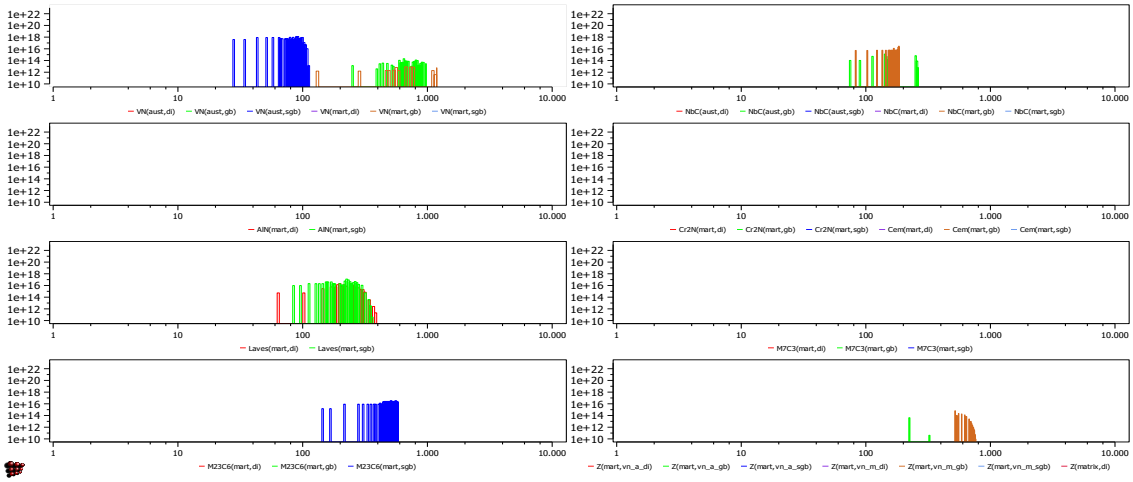

Figure C.24.: 600°C service: precipitate size classes distribution after 100 000 h

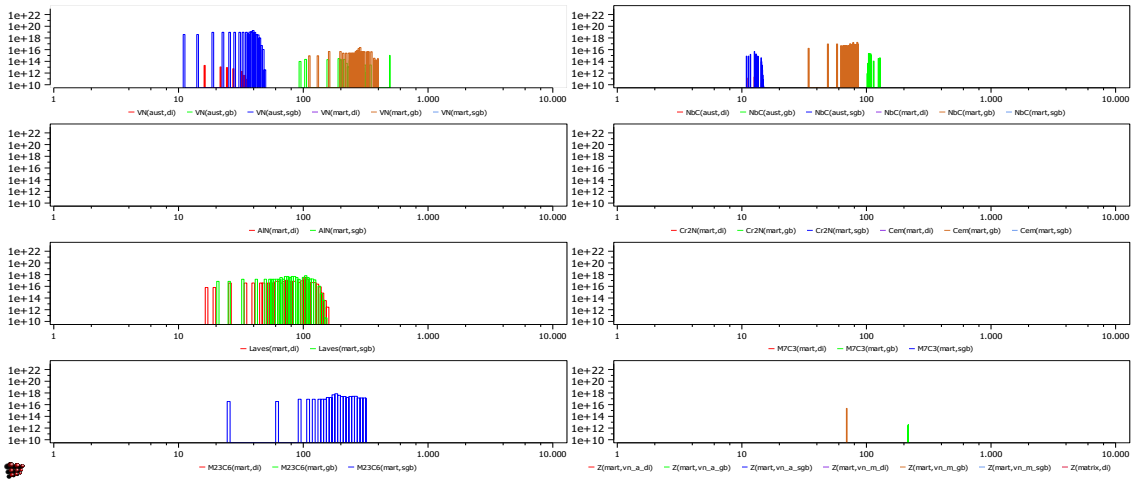

Figure C.25.: 625°C service: precipitate size classes distribution after 1 000 h

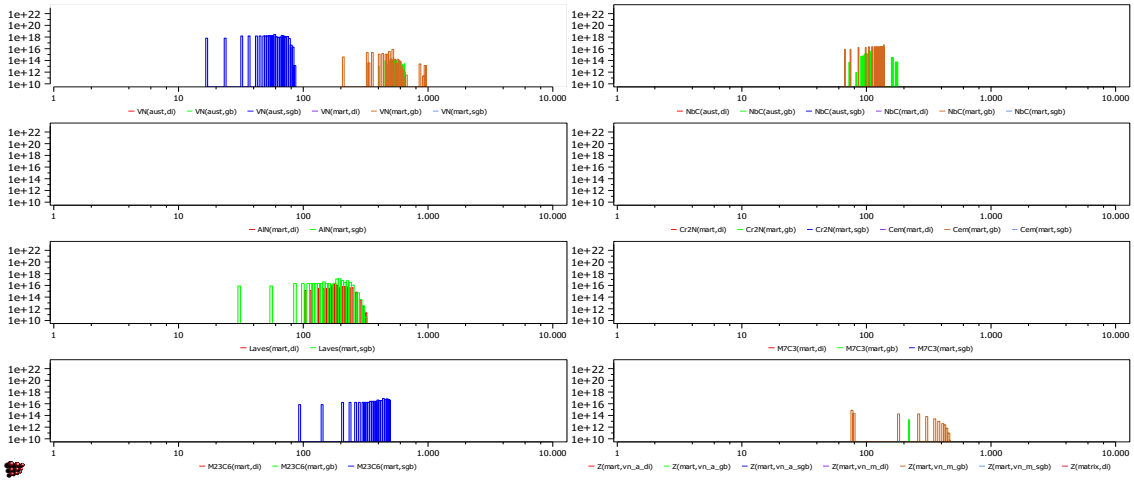

Figure C.26.: 625°C service: precipitate size classes distribution after 10 000 h

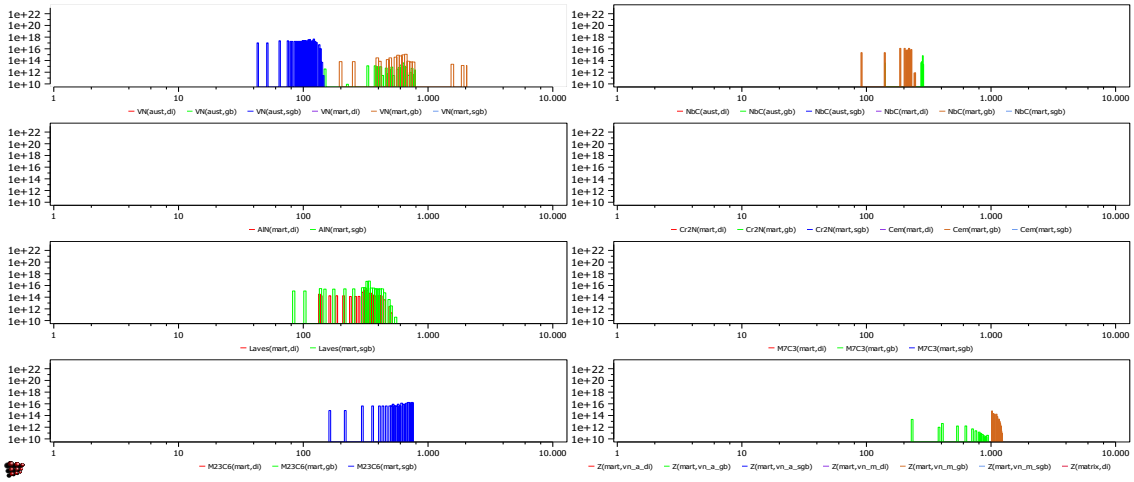

Figure C.27.: 625°C service: precipitate size classes distribution after 100 000 h

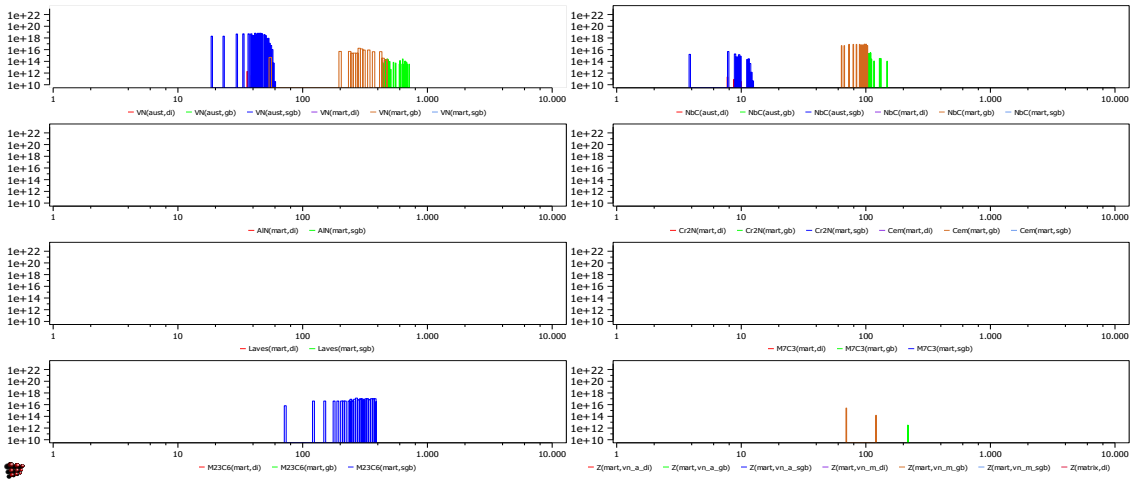

Figure C.28.: 650°C service: precipitate size classes distribution after 1 000 h

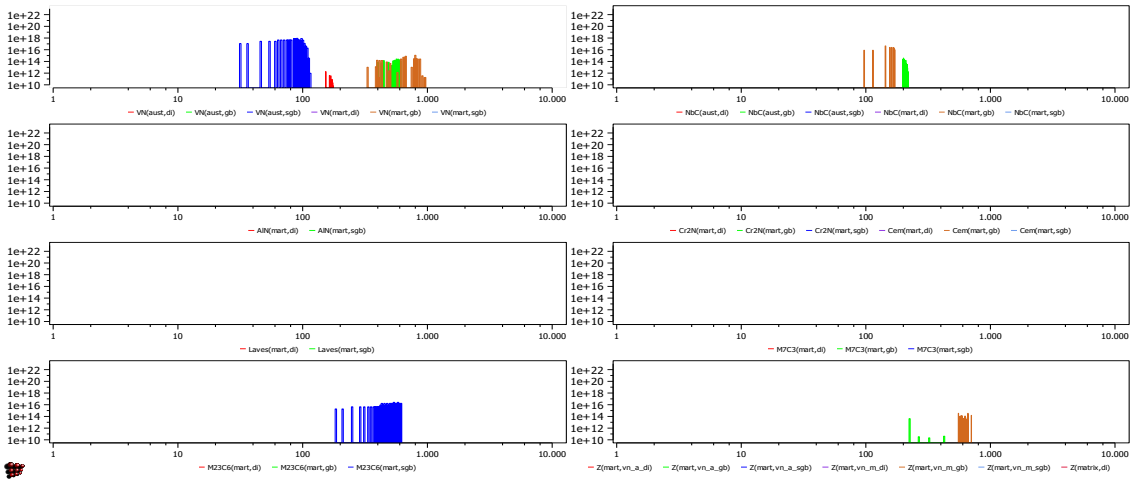

Figure C.29.: 650°C service: precipitate size classes distribution after 10 000 h

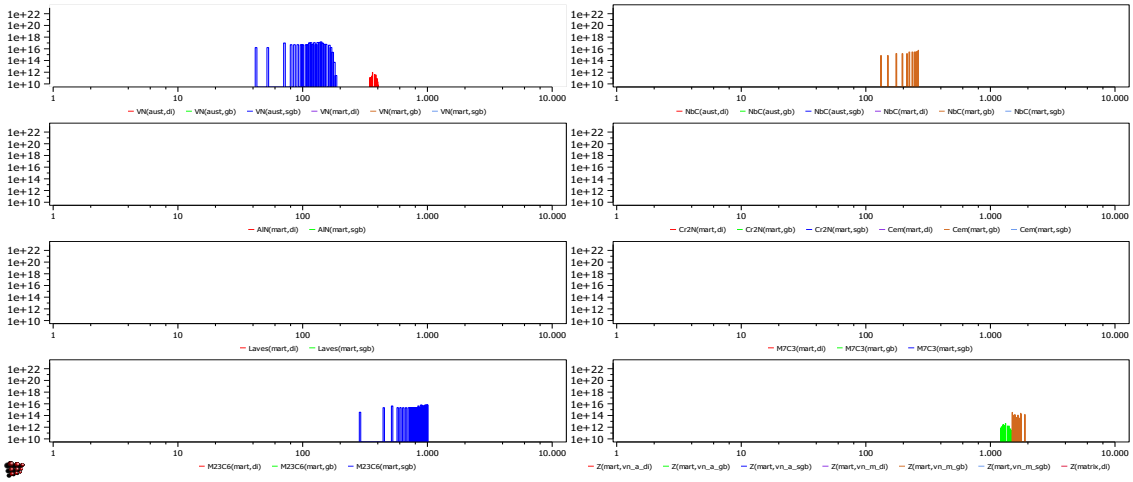

Figure C.30.: 650°C service: precipitate size classes distribution after 100 000 h