Literature study

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Outline

1. Literature
   - Precipitation
   - Dislocations
   - Metalworking techniques
2. Mathematical model
3. Integration Methods
4. Numerical results
5. Concluding remarks and future work

Literature

Focused on

- Preliminaries in metallurgy,
- Diffusion,
- Precipitation,
- Dislocations,
- Metalworking Techniques.

Precipitation

Precipitation is a reaction described by

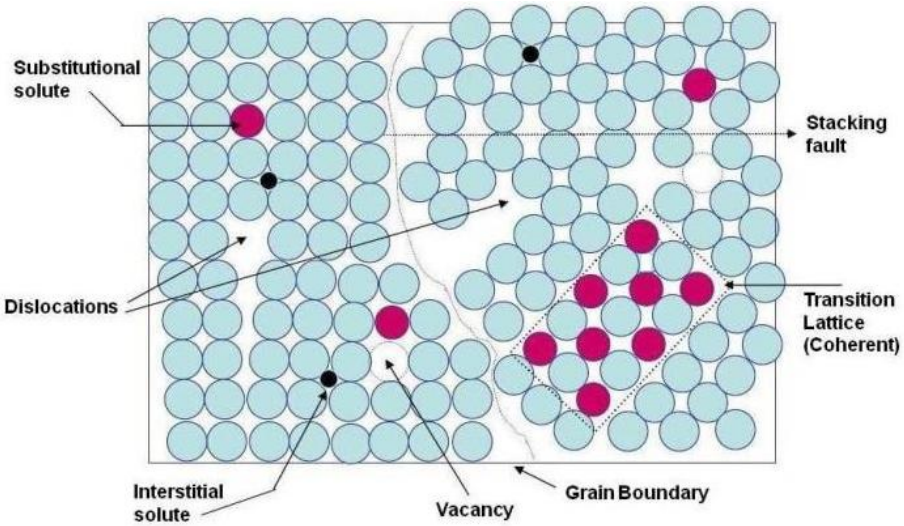
$$\alpha \rightarrow \alpha^* + \beta,$$

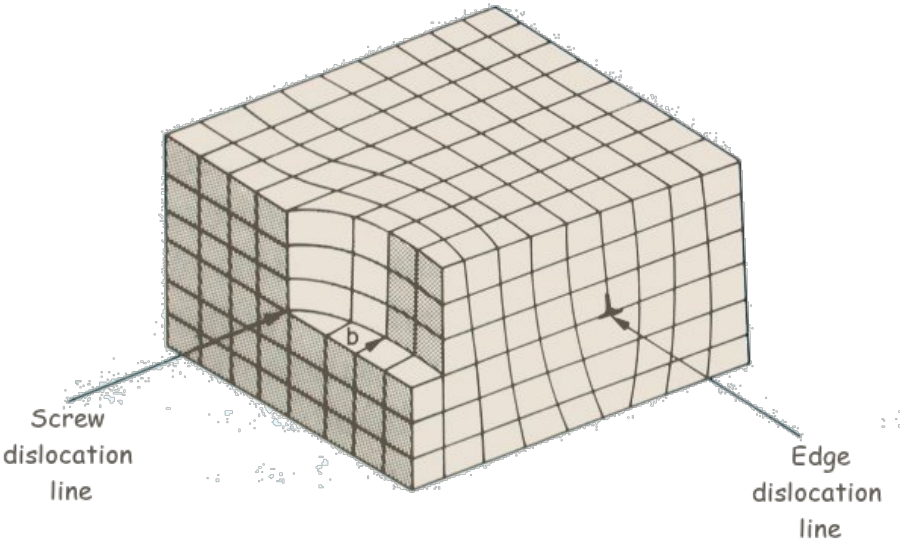
where α, α^* and β are phases
Three important concepts for precipitates

- Nucleation (homogeneous and heterogeneous)
- Growth
- Coarsening

Dislocations

We focus on heterogeneous nucleation: on defects.





Not all defects, but only dislocations.

Metalworking techniques

- Reduction of iron oxides (ore) to iron metal
- Lowering of carbon concentration and adding alloying elements
- Hot rolling of strip → **Precipitation**
- Cold rolling of strip (optional) → **Precipitation**
- Coating and painting (optional)

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   - Precipitation model
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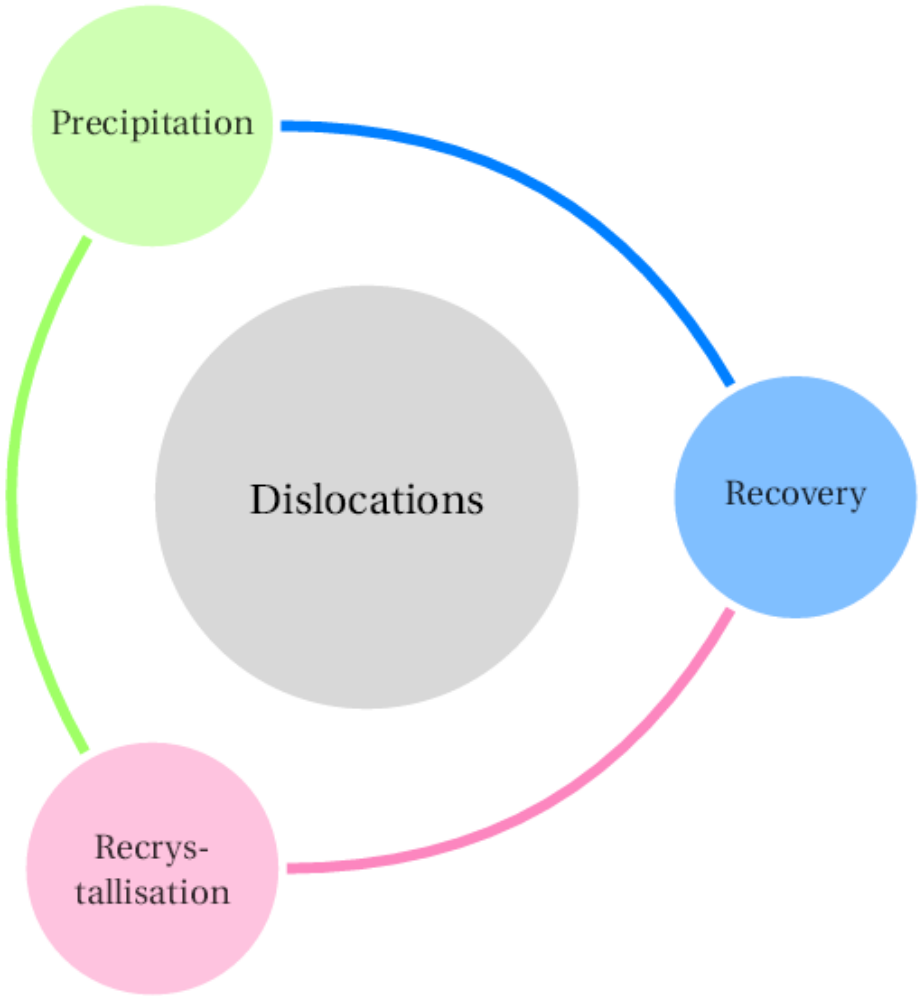
Starting point: model by Zurob et al. (2002)

Model exists of three modules:

- Precipitation
- Recovery
- Recrystallisation

which are all linked.

We focus only on the *Precipitation* model for now. (So constant dislocation density.)



Precipitation model

- Precipitation stage 1 (Nucleation and Growth)

$$\frac{dN}{dt} = \left(1 - \frac{N}{N_{total}}\right)\left(\frac{F\rho}{b}\right)\left(\frac{D_{pipe} x_{Nb}^{M}}{a^2}\right)\exp\left(\frac{-\Delta G^*}{k_b T}\right)$$

$$\frac{dR}{dt} = \frac{D_{eff}}{R}\frac{C_{Nb}^{M} - C_{Nb}^{R}}{C_{Nb}^{P} - C_{Nb}^{R}} + \frac{1}{N}\frac{dN}{dt}(\alpha_n R^* - R).$$

- Precipitation stage 2 (Growth and Coarsening)

$$\frac{dN}{dt} = F_c\left(\frac{4}{27}\frac{C_{Nb}^{Eq}}{C_{Nb}^{P} - C_{Nb}^{Eq}}\frac{R_0 D}{R^3}\right)\left(\frac{R_0 C_{Nb}^{M}}{R(C_{Nb}^{P} - C_{Nb}^{M})}\left(\frac{3}{4\pi R^3} - N\right) - 3N\right)$$

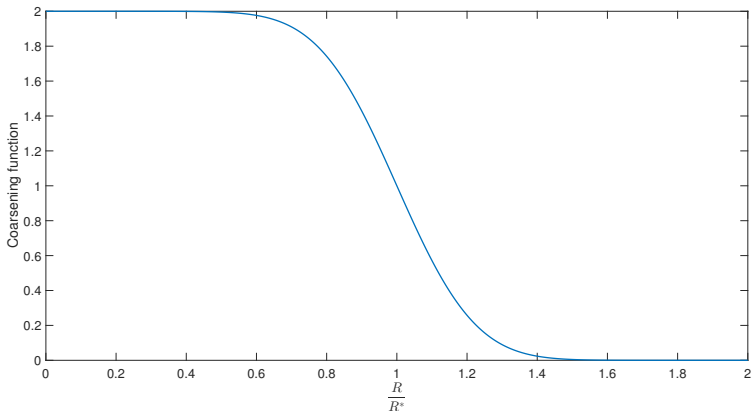
$$\frac{dR}{dt} = (1 - F_c)\left.\frac{dR}{dt}\right|_{\text{growth}} + F_c\left.\frac{dR}{dt}\right|_{\text{coarse}}$$

Coarsening function

- Critical radius for homogeneous nucleation

$$F_c = 1 - \mathrm{erf}\left(4\left(\frac{R}{R_0}\ln\left(\frac{C_{Nb}^{M}}{C_{Nb}^{Eq}}\right) - 1\right)\right) = 1 - \mathrm{erf}\left(4\left(\frac{R}{R_h^*} - 1\right)\right),$$

- Takes values between 2 and 0, instead of between 1 and 0



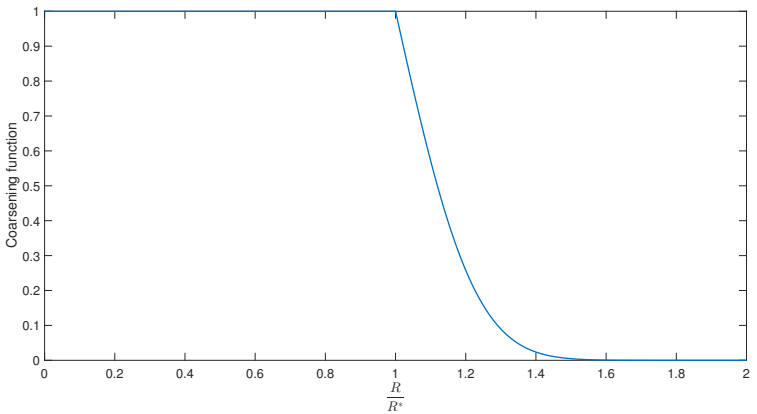


Figure: Deschamps' coarsening function F_c against R/R^*.

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Integration methods

Requirements for the integration method

- Large time steps
- Short computation times
- Simple implementation

TATA Steel uses the explicit, fourth order Runge-Kutta method. We choose

- Backward Euler method
- Backward Euler with Forward Euler method
- Blackbox algorithm from MATLAB

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4. Numerical results
   - Integration methods
   - Coarsening function
   - Variable variation
5. Concluding remarks and future work

Standard settings

The standard setting as used in the simulations

Table: Precipitation parameters.

Parameter	Value	Unit
T	1123.15 (850 °C)	K
ρ	3.27×10^{14}	$1/\mathrm{m}^2$
$N(0)$	1×10^{10}	$1/\mathrm{m}^3$
$R(0)$	R^*	m

Table: Numerical parameters.

Parameter	Value	Unit
F	1.32×10^{-3}	
t_{start}	0.001	s
t_{end}	12040	s

Table: Alloy composition of alloy N1 in weight percentages .

C	Si	Mn	P	S	Nb	Al	N	Fe
0.076	0.06	1.34	0.0058	0.0026	0.03	0	0.0061	93.3815

For our alloy we have a R^* of 2.49×10^{-10}.

Variation of functions and parameters

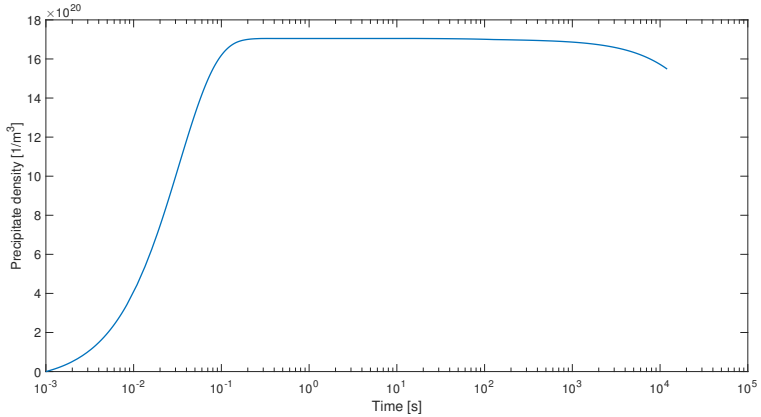
We perform simulations for different

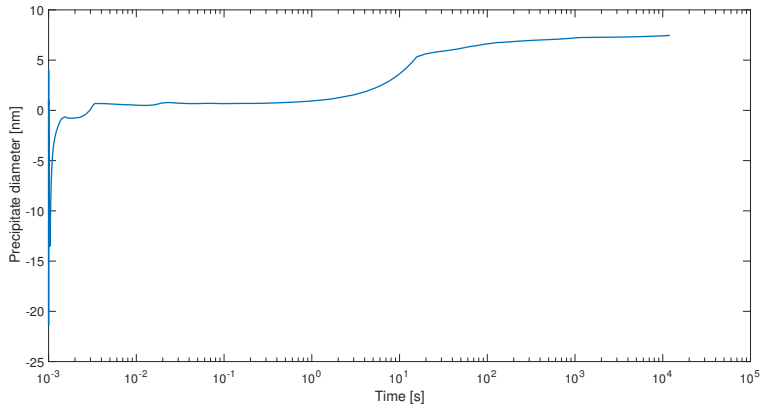
- Integration methods
- Coarsening functions
- Initial and model variables
  - Initial precipitate number density and precipitate mean diameter
  - Temperature, both isothermal and non-isothermal calculation
  - Dislocation densities
  - Chemical compositions

Integration methods

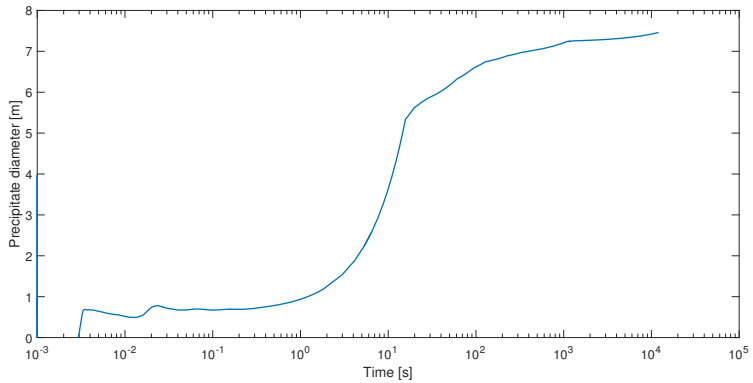
- Backward Euler method
- Backward Euler with Forward Euler method
- Blackbox algorithm from MATLAB

Blackbox algorithm from MATLAB





- Precipitate mean diameter not smooth
- Precipitate mean diameter physically unacceptable results



Integration methods

- Backward Euler method
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Integration methods

- Backward Euler method
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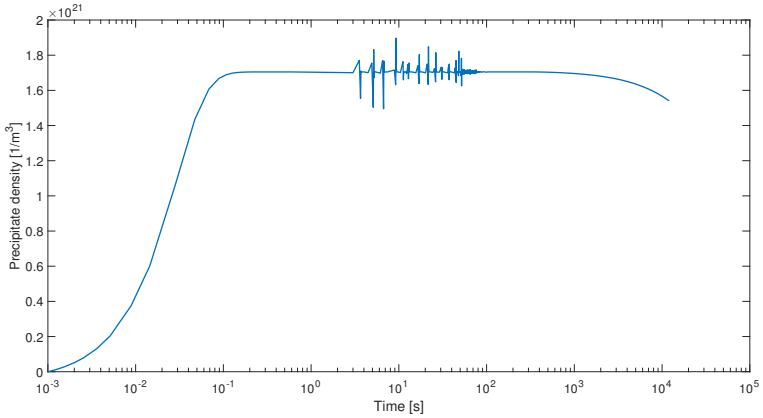
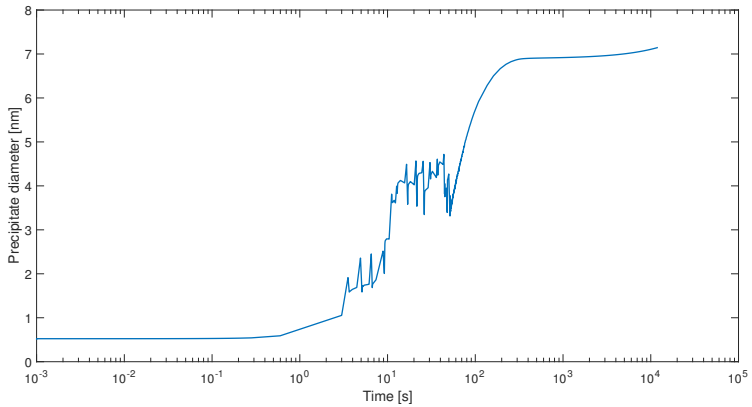
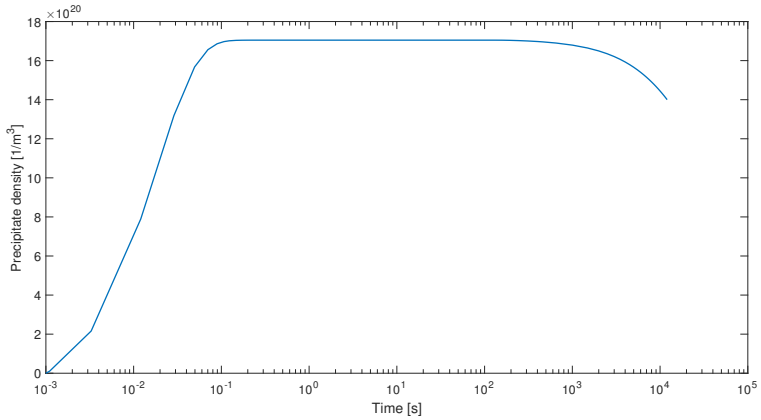
Backward Euler with Forward Euler method

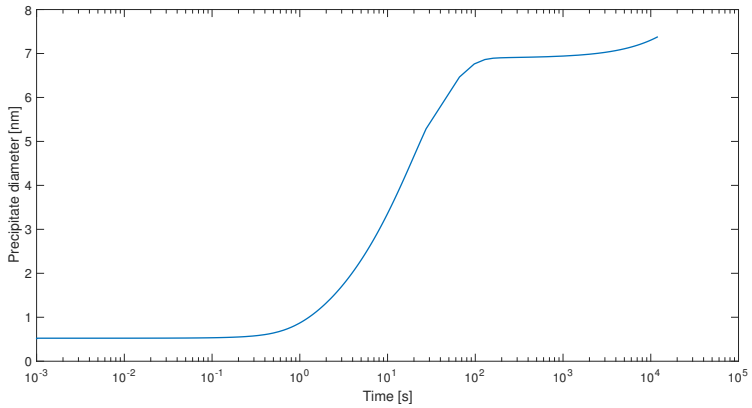




- Oscillations due to the forward step.

Backward Euler method





- Smooth solution, except bend in precipitate number density
- Coarsening clearly visible

Integration methods

- Backward Euler method
- Backward Euler with Forward Euler method
- ~~Blackbox algorithm from MATLAB~~

Integration methods

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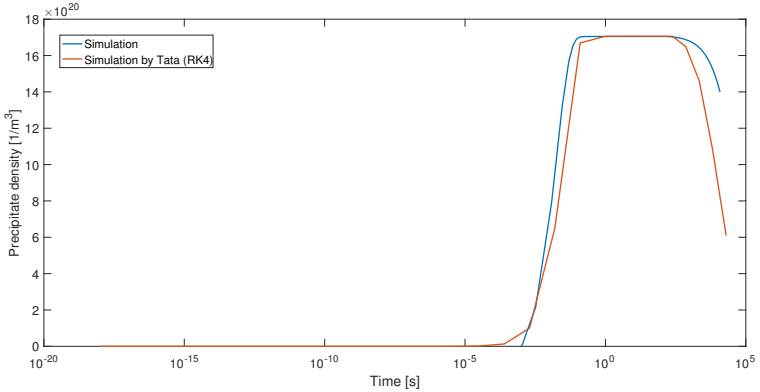
Simulations Tata Steel and literature study

Simulation results using BE compared to simulation by Tata Steel using Runge-Kutta 4



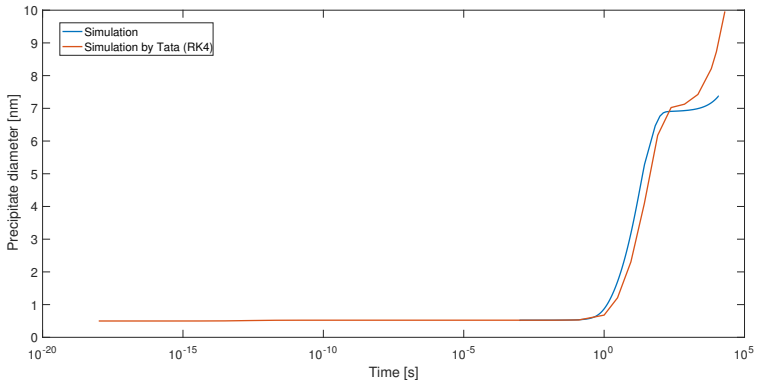


Table: Differences in implementation between this literature study and Tata Steel

Literature Study	Tata Steel
Backward Euler	Runge-Kutta 4
$\frac{dR}{dt} = \frac{4}{27} \frac{C_{Nb}^{Eq}}{C_{Nb}^{P} - C_{Nb}^{Eq}} \frac{R_0 D}{R^2}$	$\frac{dR}{dt} = \frac{D_{eff}}{R} \frac{0.01(wt\%Nb^{R} - wt\%Nb^{R27/23})}{wt_{Nb}^{P} - 0.01 wt\%Nb^{Eq}}$
Concentrations	Weight percentages / molar fractions

Coarsening function

1. The original coarsening function with the heterogeneous or homogeneous critical radius and restrictions proposed by Kranendonk (2005):

$$F_c = 1 - \mathrm{erf}\left(4\left(\frac{R}{R^*_{(h)}} - 1\right)\right).$$

2. A coarsening function based on the current volume fraction (f_v) and the equilibrium volume fraction corrected by the Gibbs-Thomson effect ($f_{v,GT}$) by Perrard et al. (2007):

$$F_c = \sup\left[1 - 100\left(\frac{f_v}{f^{eq}_{v,GT}} - 1\right)^2, 0\right].$$

Coarsening functions in time

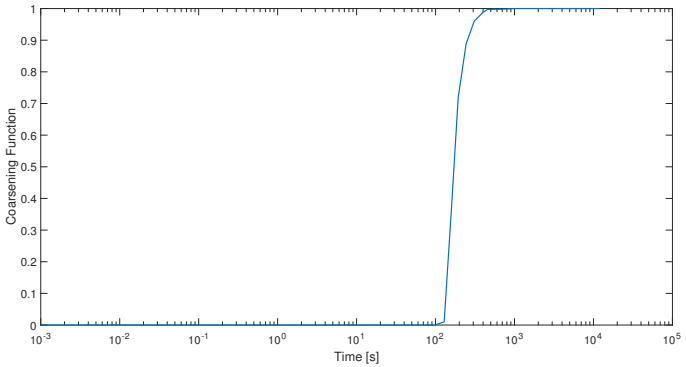


Figure: By Deschamps

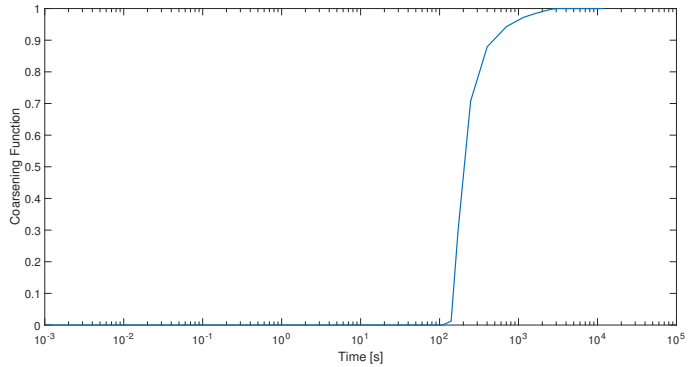


Figure: By Kranendonk.

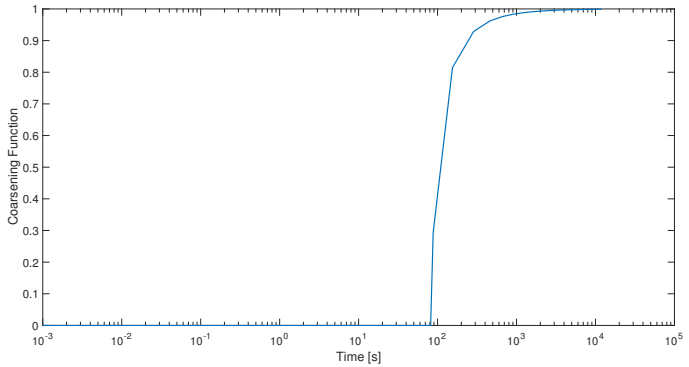
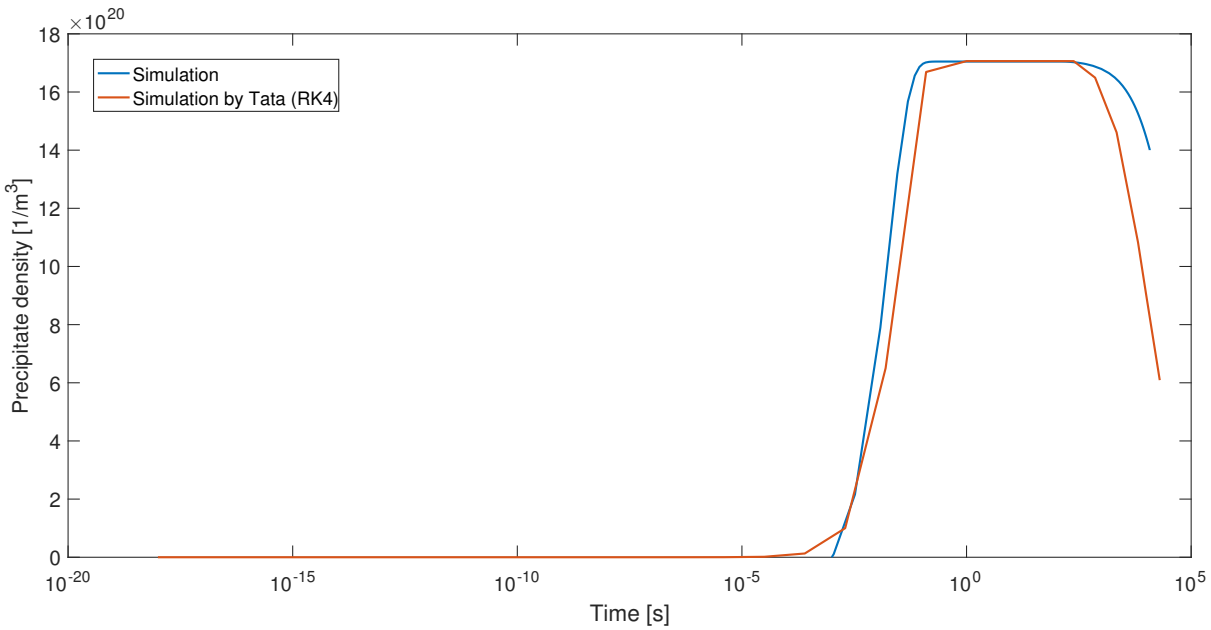


Figure: By Perrard.

Initial density and mean radius

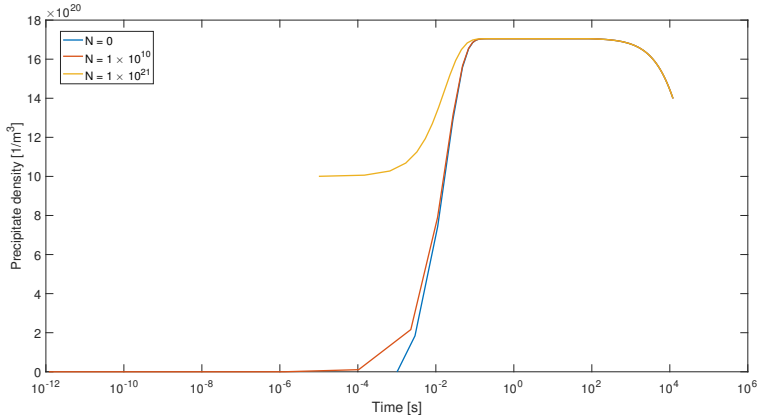
Simulation with , at $t = 0$:

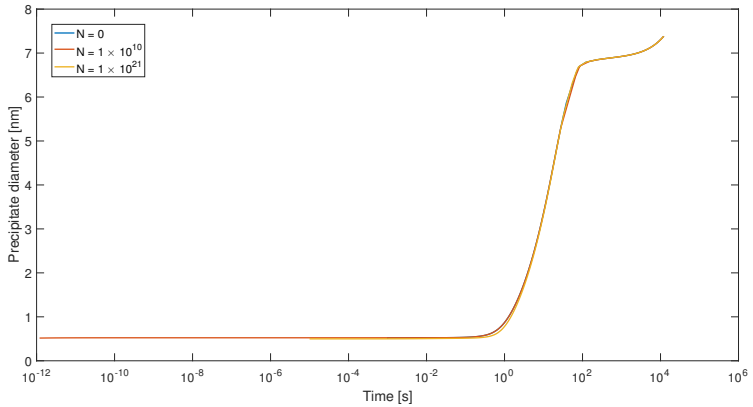
- $N(0) = 0$, $R(0) = R^*$
- $N(0) = 1 \times 10^{10}$, $R(0) = R^*$
- $N(0) = 1 \times 10^{21}$, $R(0) = R^*$

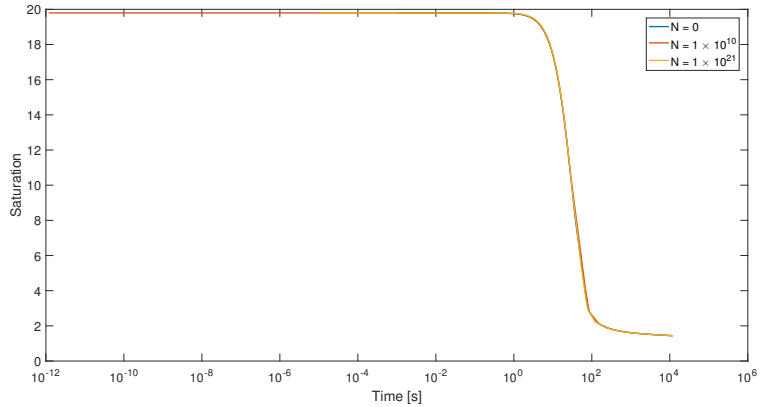


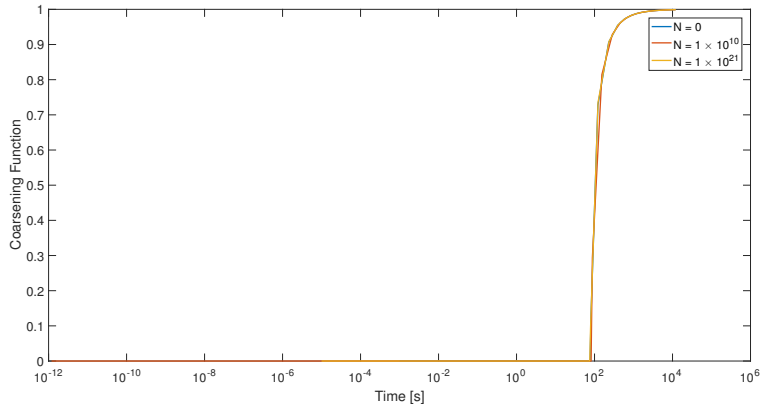
Simulation results at 850 °C and $\rho = 3.27 \times 10^{14}$ m^{-2}.

Initial density and mean radius - Simulation results







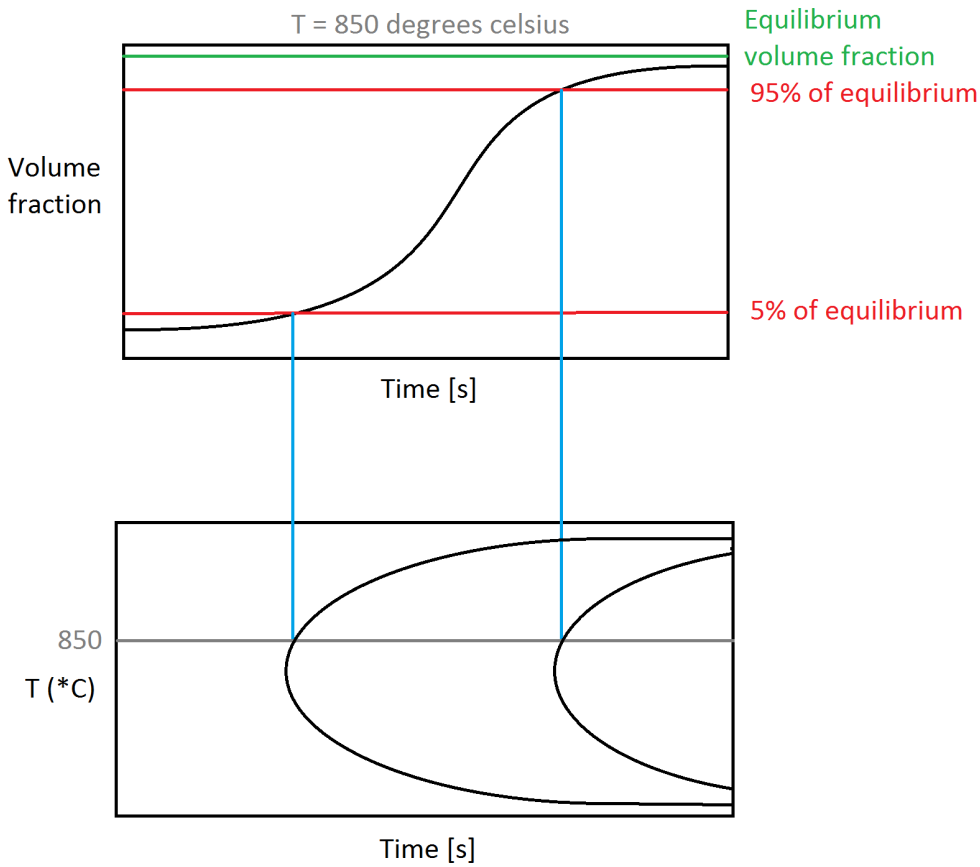


Temperature

Restrictions on the chosen temperature

- Restrict the simulations to austenite (min. ± 700 °C)
- Stay below the solvus temperature (max. 1093.88 °C for chosen alloy)

Using the results for different isotherm calculations we construct a Precipitate-Time-Temperature diagram.



Temperature

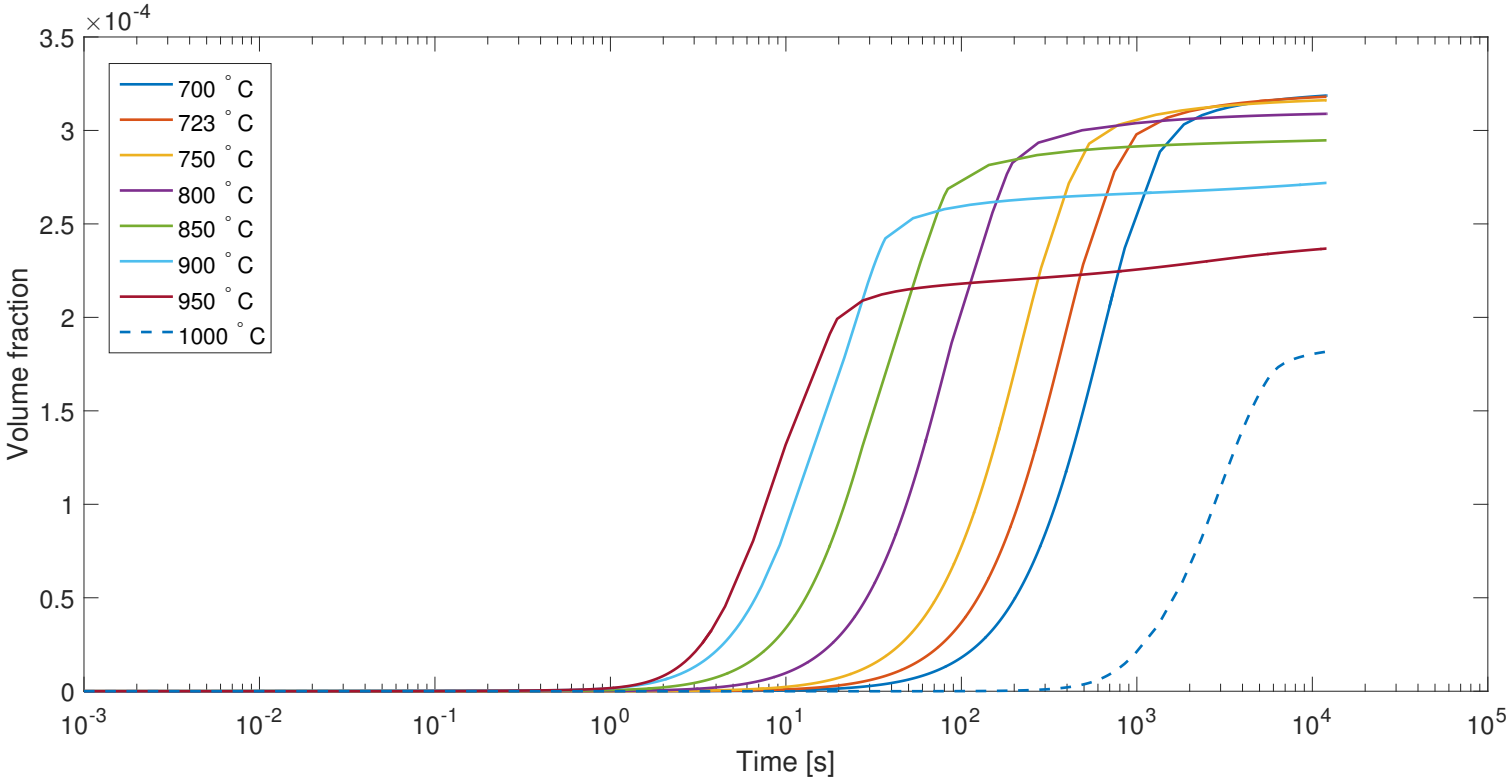


Figure: Volume fraction in time for different temperatures with $\rho = 3.27 \times 10^{14}$ m^{-2}.

Temperature

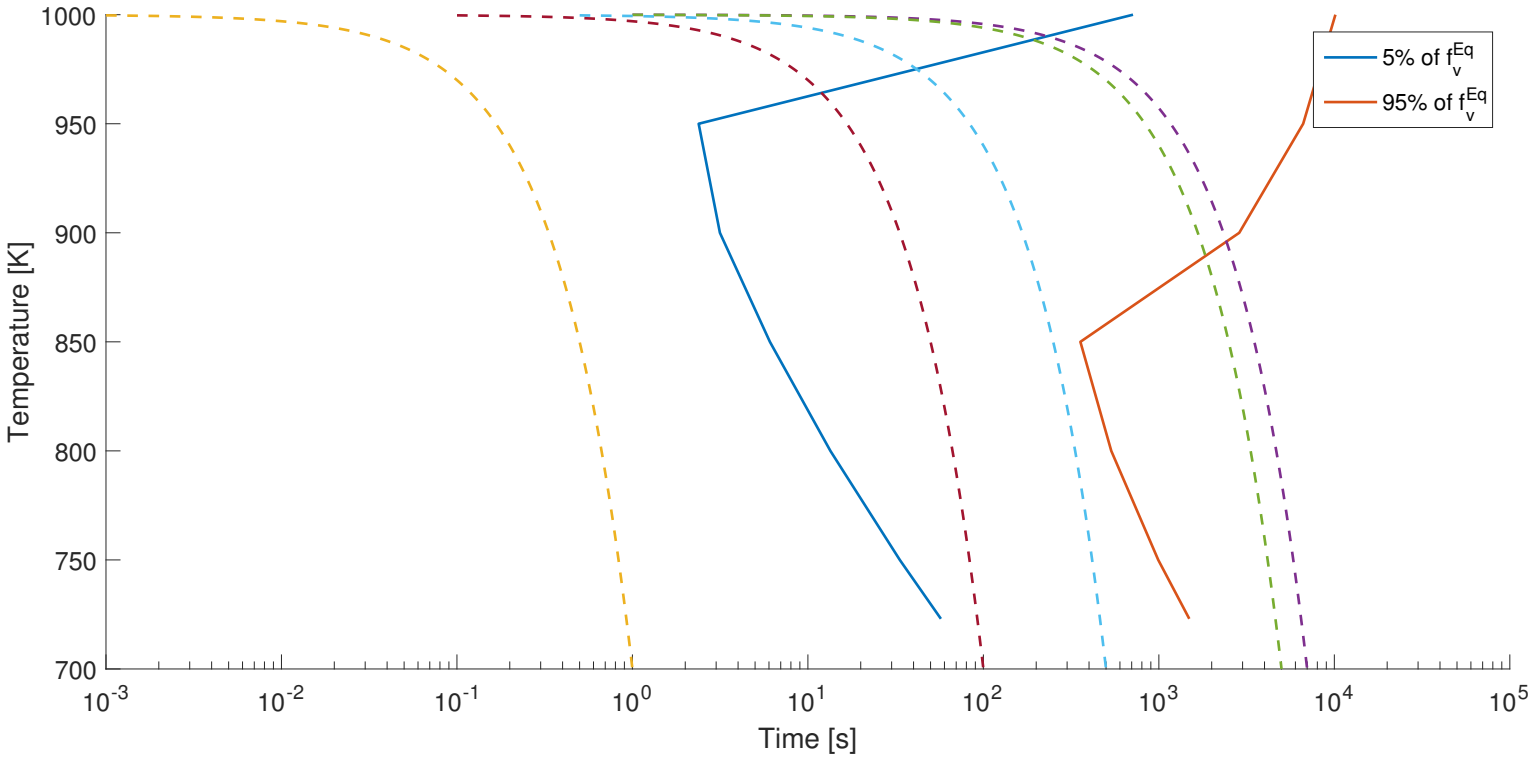
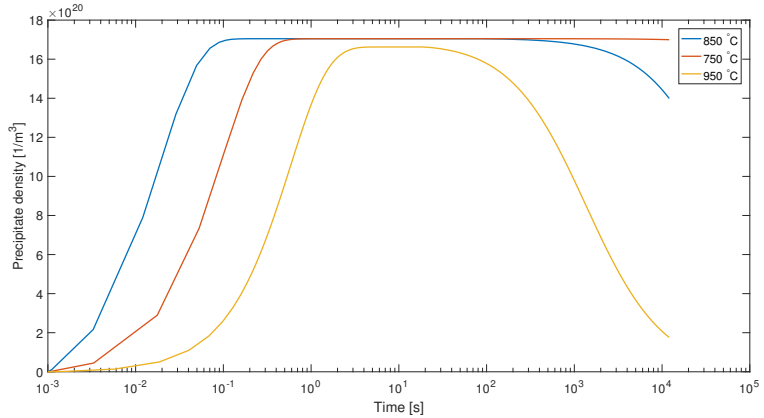
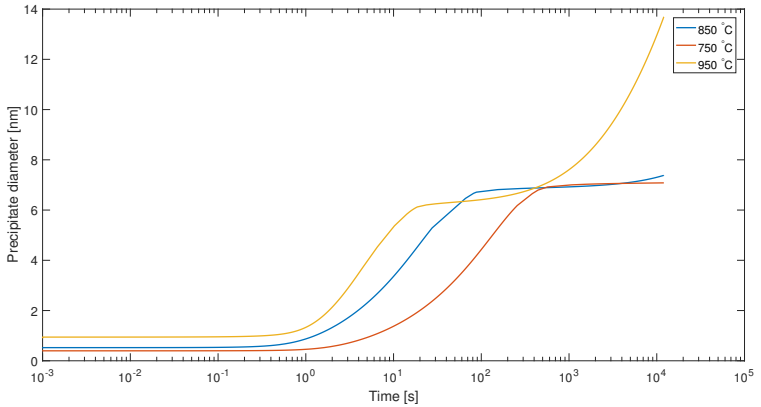
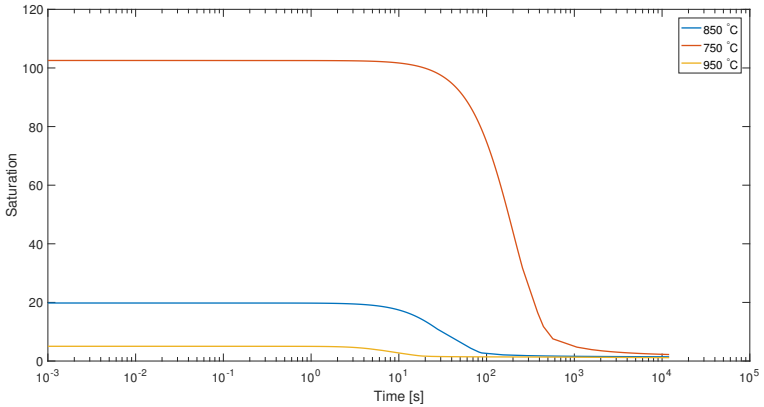


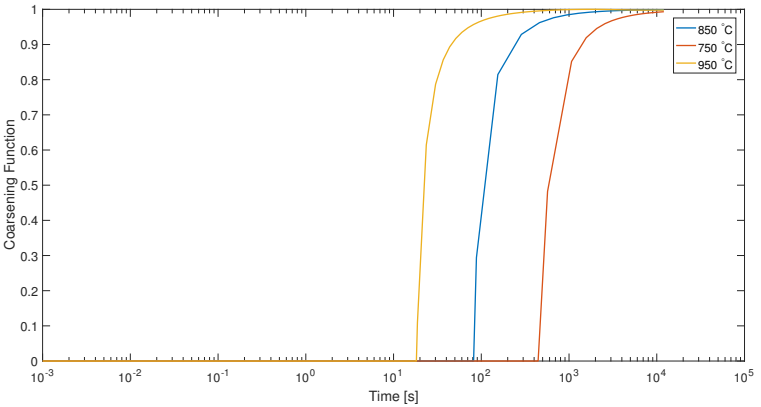
Figure: Precipitate-time-temperature curve on a logarithmic time scale and various temperature cooling curves.

Temperature - Simulation results ($\rho = 3.27 \times 10^{14}$ m^{-2})



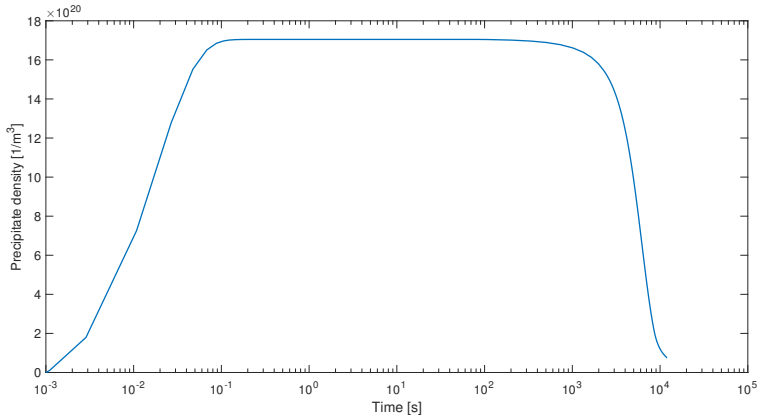


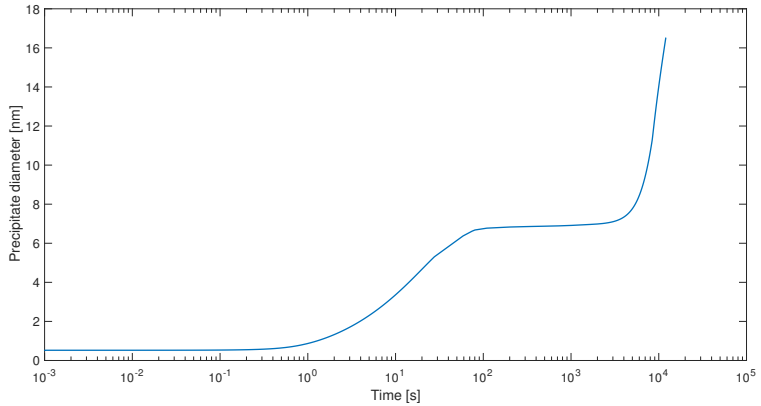


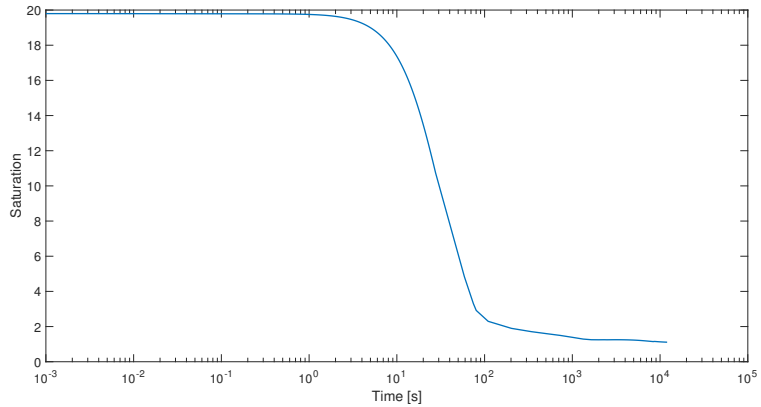


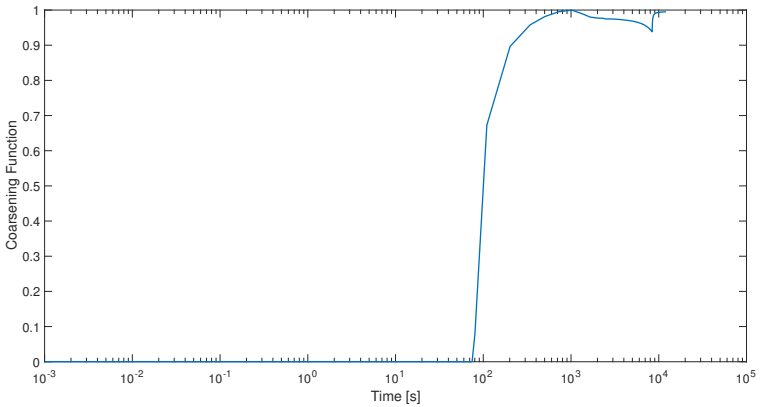
Non-isotherm calculations

Linear temperature increase from 850 °C to 1000 °C in in 140 minutes, after which the temperature stays constant.









Volume fraction

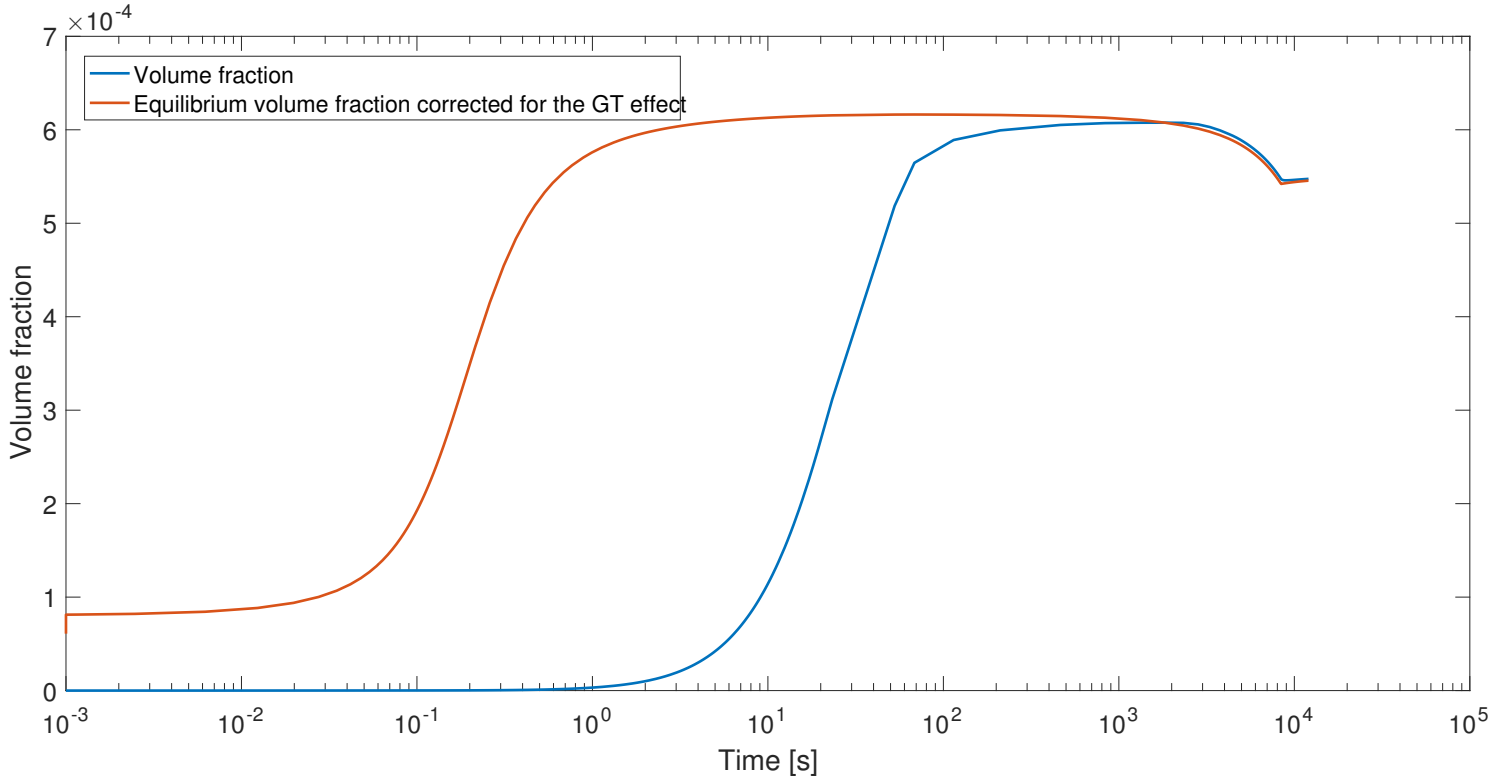


Figure: Volume fraction and equilibrium volume fraction corrected for the Gibbs-Thomson effect in time with a linear temperature increase and $\rho = 3.27 \times 10^{14}$ m^{-2}.

Dislocation density

Simulations with

- 3.27×10^{14} m^{-2}, the original dislocation density from previous simulations,
- 1.18×10^{14} m^{-2}
- 6.54×10^{14} m^{-2}

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The dislocation density ρ occurs twice in the precipitation model.

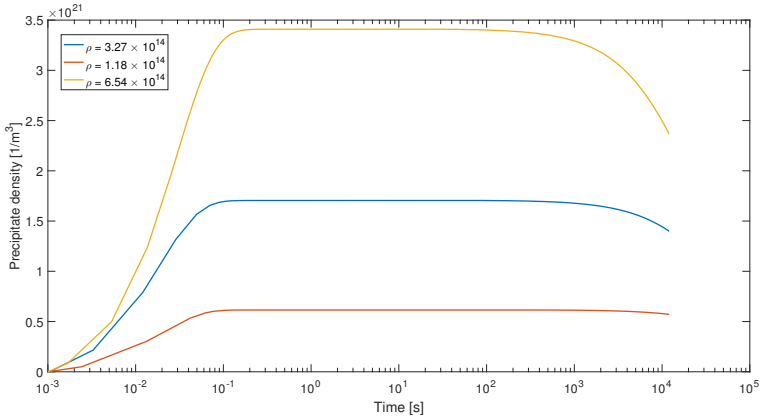
1. In the maximum number of potential nucleation sites N_{total}

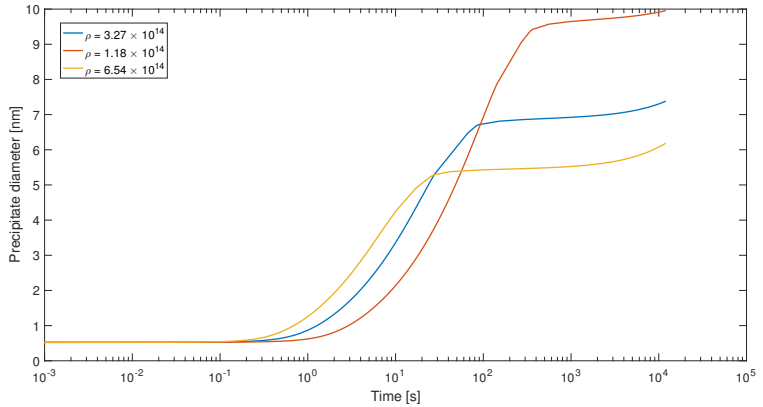
$$N_{total} = \frac{F\rho}{b}.$$

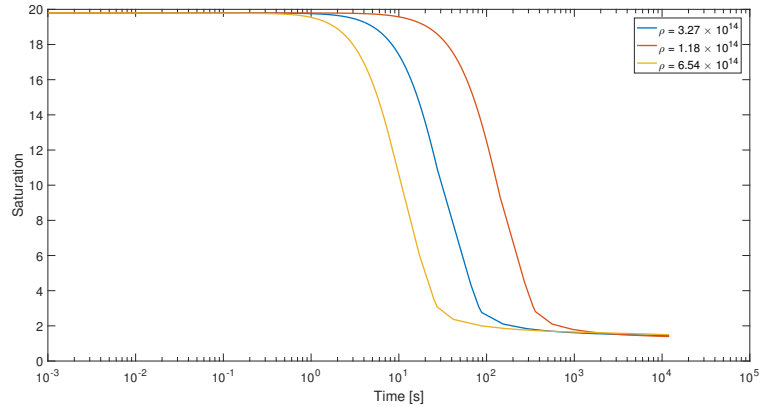
2. In the effective diffusion coefficient D_{eff}

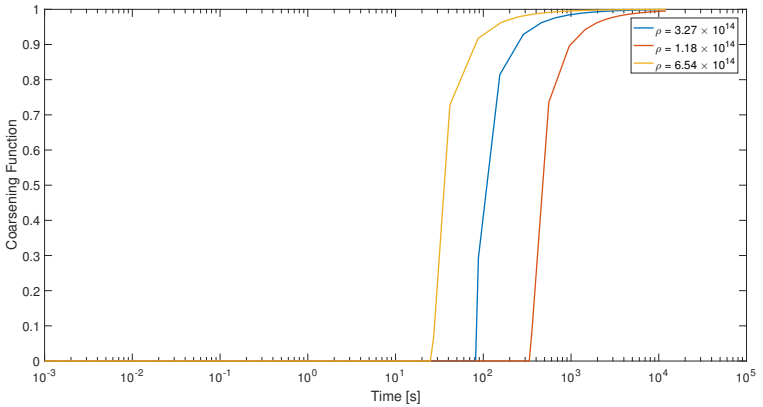
$$D_{eff} = D_{pipe}\pi b^2 \rho + D_{bulk}(1 - \pi b^2 \rho).$$

Dislocation density - Simulation results (850 °C)









Chemical composition

Element with lowest molar fraction determines the maximum volume fraction.

Table: Initial weight percentages and fractions of the precipitate elements.

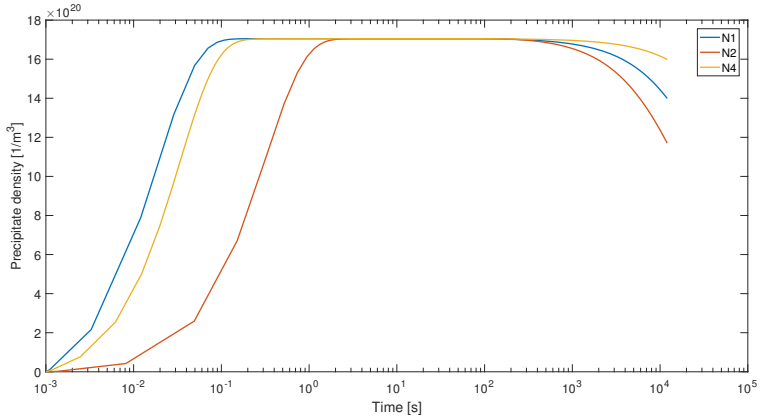
Alloy	Nb	C	N	X_{Nb}	X_C	X_N
N1	0.03	0.076	0.0061	1.7947×10^{-4}	0.0035	2.4201×10^{-4}
N2	0.007	0.20	0.0056	4.1628×10^{-5}	0.0092	2.2085×10^{-4}
N4	0.058	0.21	0.0061	3.4488×10^{-4}	0.0097	2.4054×10^{-4}

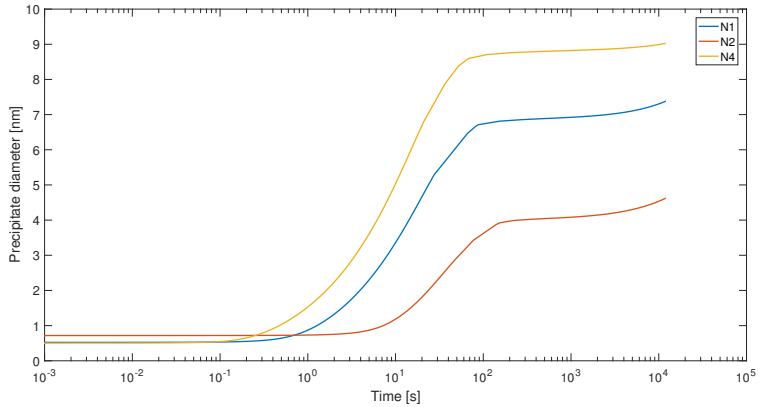
$$f_v = \frac{4}{3}\pi N R^3$$

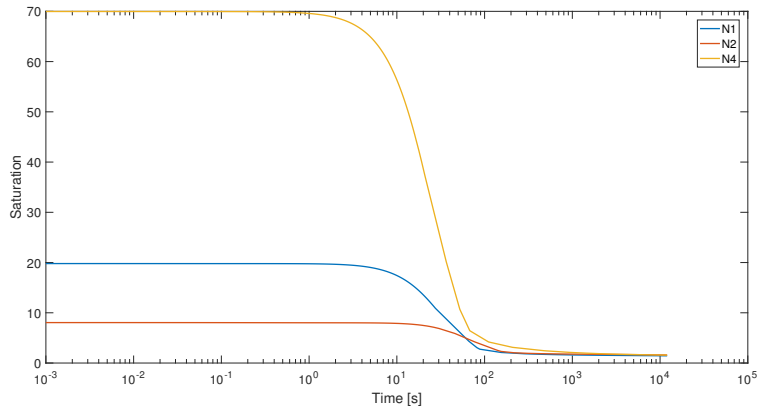
At equal dislocation density: a higher volume fraction leads to larger precipitates.

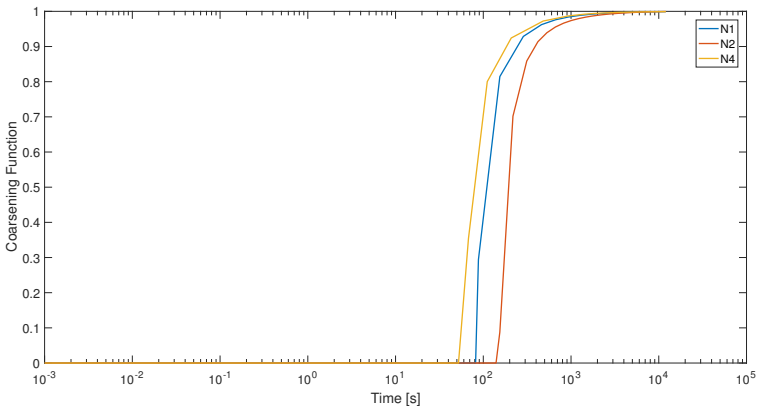
Simulation results at 850 °C and $\rho = 3.27 \times 10^{14}$.

Chemical composition - Simulation results









Outline

1. Literature
2. Mathematical model
3. Integration Methods
4. Numerical results
5. Concluding remarks and future work
   - Concluding remarks
   - Future work

Concluding remarks

The results using the precipitation model by Zurob seem to be realistic and predict the experimental data quite well after fitting.

For applications to modern steel grades a number of improvements and extensions is needed:

- Physical approximations in the model
- Different precipitates can not be modelled simultaneously
- Use of the mean radius of the precipitate
- No homogeneous nucleation

Future work

- Make a new model with distributions, based on the old model.
- Improve the new model with a multi-component version.
- Improve the physical approximations made in the new model.
- Couple the new model to the recrystallisation and recovery models.
- Improve the recrystallisation and recovery model.
- Add the homogeneous precipitation model to the system.

Literature study

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