Effect of thermodynamic conditions at the interface on the ferrite formation kinetics in steels with inhomogeneous chemical composition

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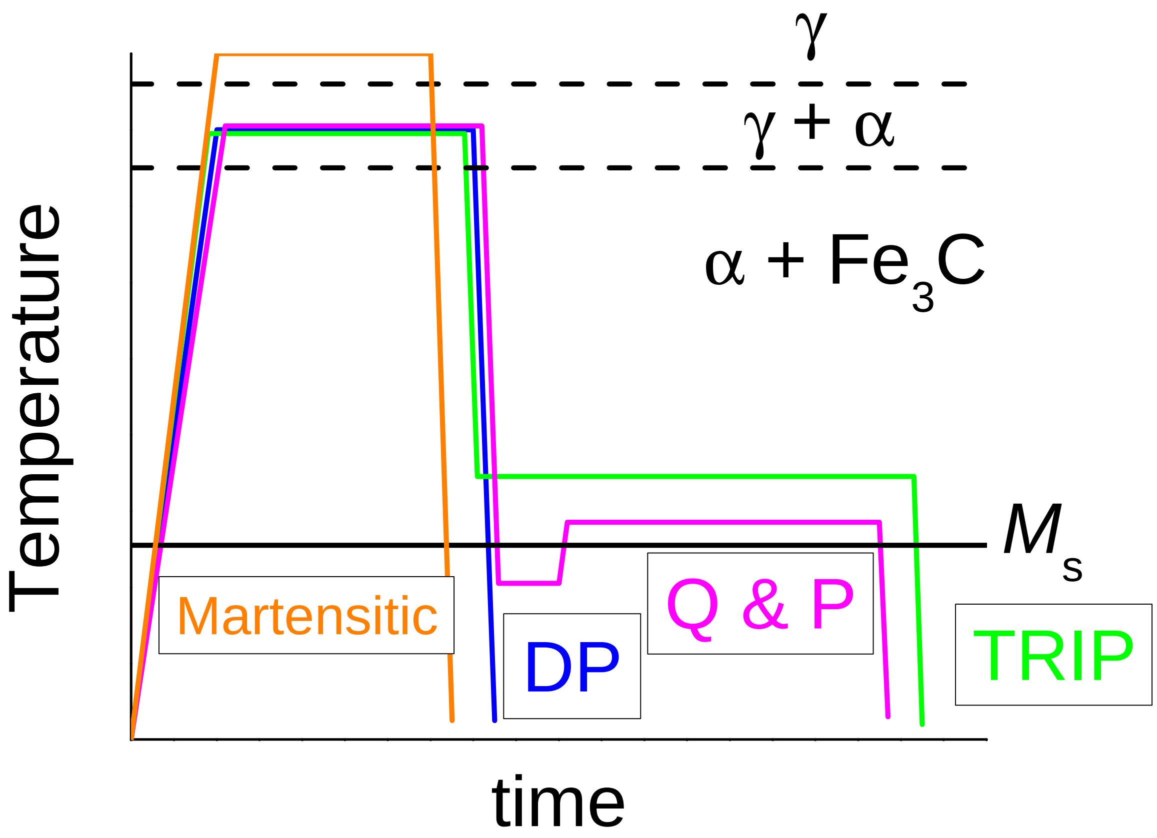
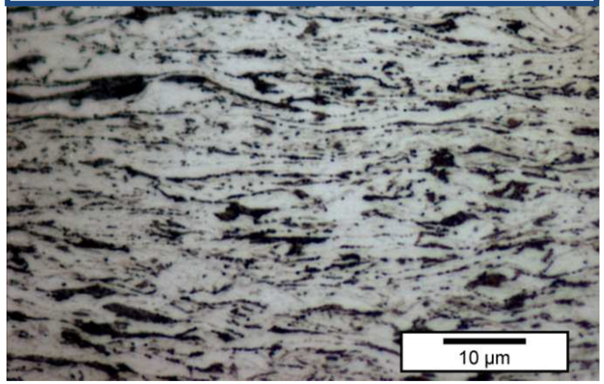
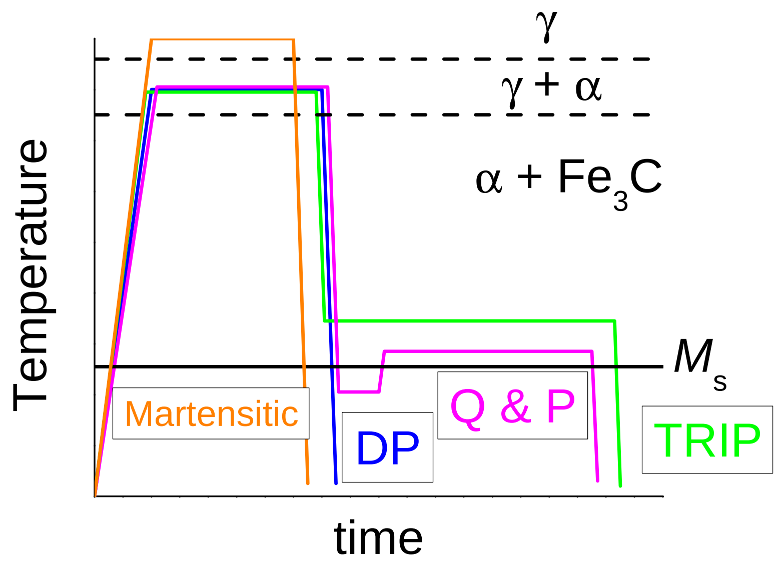
Background

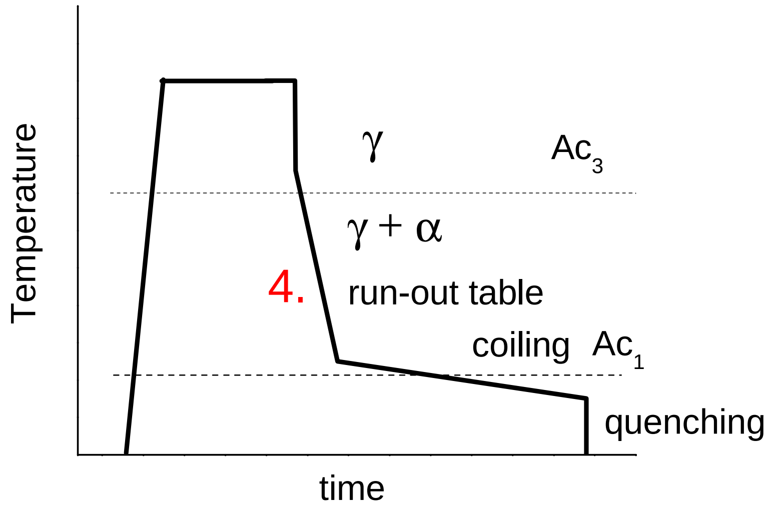


Background

Microstructural banding







Recrystallisation and austenite formation,
Ferrite, carbides, bainite and martensite formation

Austenite to ferrite in presence inhomogeneous Mn composition

Background

Physical-based model to link the process setting with the final microstructure & properties of the steel

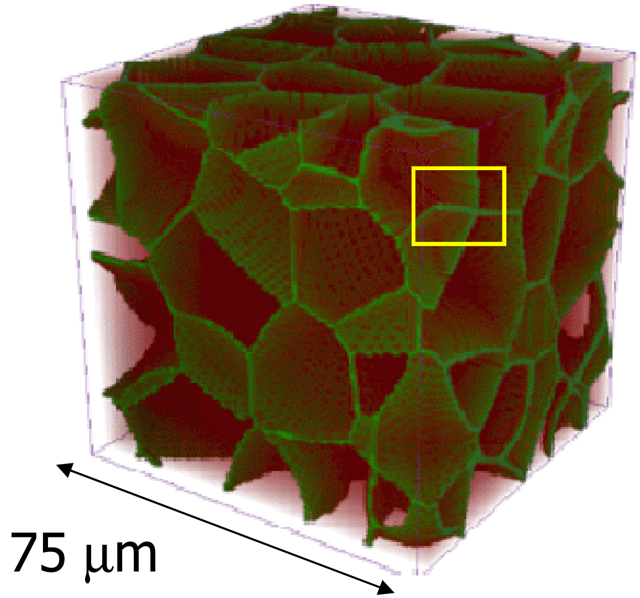
Phase field model

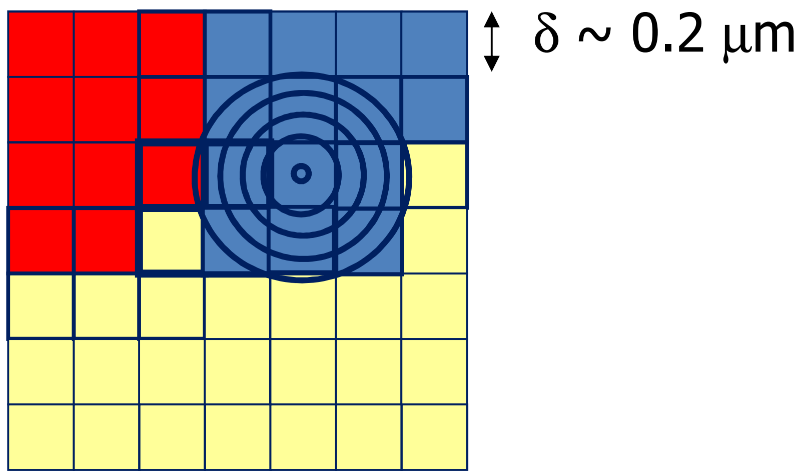
3D mixed-mode model

Outline

- 3D mixed mode sharp interface model
  - Cellular automata (CA) algorithm
  - Nucleation and growth model
  - Thermodynamic condition at the interface
- Material and experimental data
- Model validation

3D microstructure model: *CA algorithm*





1. The grain to which the cell belongs

2. The growth parameter $$l^i_{cell}(t+\Delta t) = l^i_{cell}(t) + v^i_{cell}\,\Delta t$$

$v^i_{cell} \Rightarrow$ grain boundary velocity, v

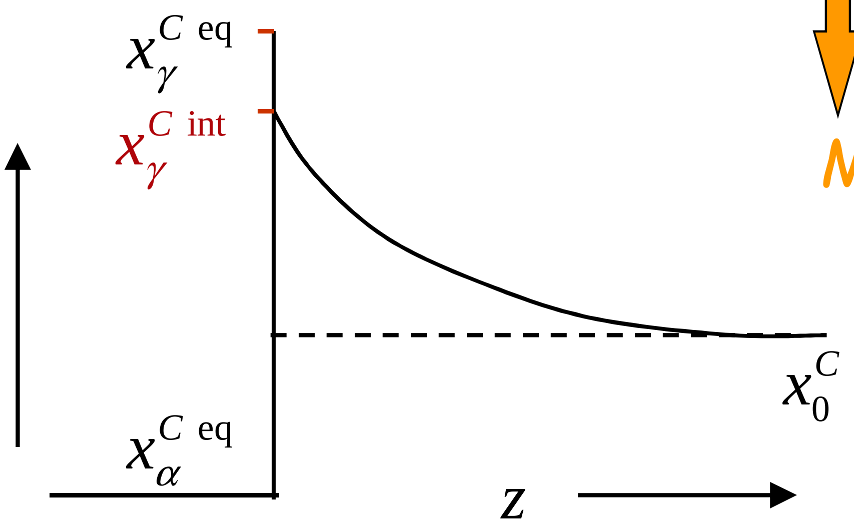
3D microstructure model: ferrite growth

$$v^{\alpha\gamma} = M^{\alpha\gamma}\ \Delta G_{\alpha\gamma}\left(x_C^{\gamma,\mathrm{int}}, x_{Mn}^{\gamma}\right)$$

$$M_0^{\alpha\gamma}\exp\left(-Q^{\alpha\gamma}/RT\right)$$

Local Mn content

Mixed-mode model [1]



1. K. Bos, J. Sietsma, Scripta Mater. 57 (2007) 1085

3D microstructure model: ferrite growth

$$\Delta G = \sum_{k=1}^{N} x_k^{\alpha} \left(\mu_k^{\gamma} - \mu_k^{\alpha} \right)$$

- The composition of the parent and new phase is used to calculate the chemical potential via the TQ-interface of Thermo–Calc® software

- Mixed-mode condition for the interstitial element (C)
- Negligible or without partition for the substitution element (Mn)

Mixed mode negligible partitioning (MMNP)

Mixed mode without partitioning (MMWP)

3D microstructure model:
ferrite nucleation

$$\frac{dN}{dt} = K_N \frac{k_B T}{h} exp\left(-\frac{Q_d}{k_B T}\right) exp\left(-\frac{\Delta G^*}{k_B T}\right)$$ [1]

$$\Delta G^* = \frac{\Psi}{\Delta G_v^{\,2}} \qquad \Delta G_v = \chi_T (T_{Ae3} - T)$$

$T_{Ae3} \rightarrow x_C^{\gamma},\ x_{Mn}^{\gamma}$

$$\frac{dN}{dt} = K_N \frac{k_B T}{h} \exp\left(-\frac{Q_d}{k_B T}\right) \exp\left(-\frac{L}{k_B T (T_{Ae3} - T)^2}\right)$$

$$L = \frac{\Psi}{\chi_T^{\,2}}$$

1. S.E. Offerman et al, Mat.Sci. Techn. 18 (2002) 297

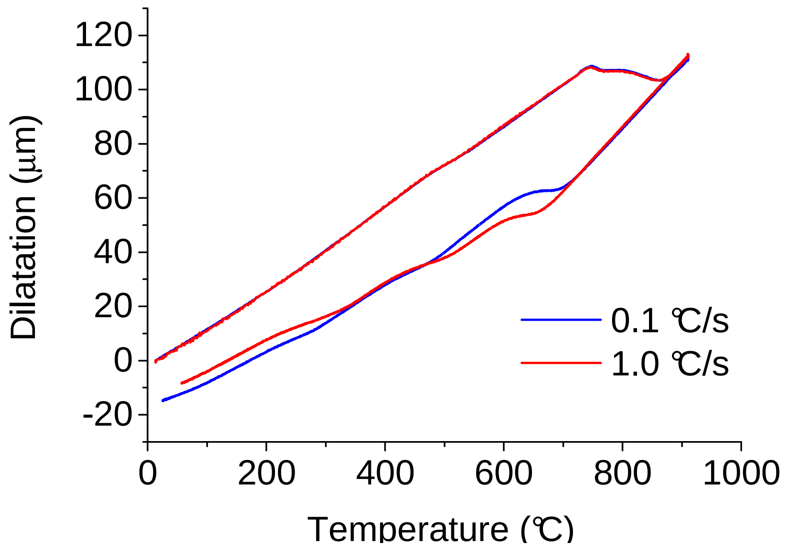
3D microstructure model:
ferrite nucleation

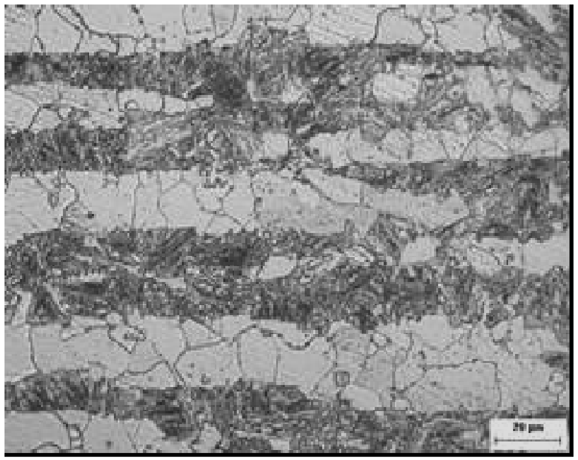
$P = \Delta t \frac{\mathrm{d}N}{\mathrm{d}t}$ probability that a nucleation site becomes active

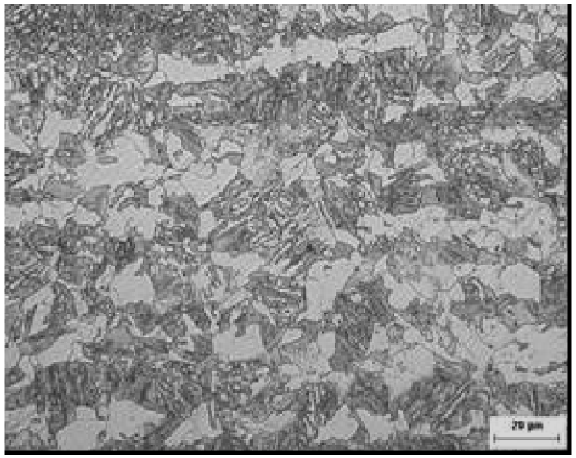
if $R < P$ (R random number) nucleation site becomes active

Material and experimental results

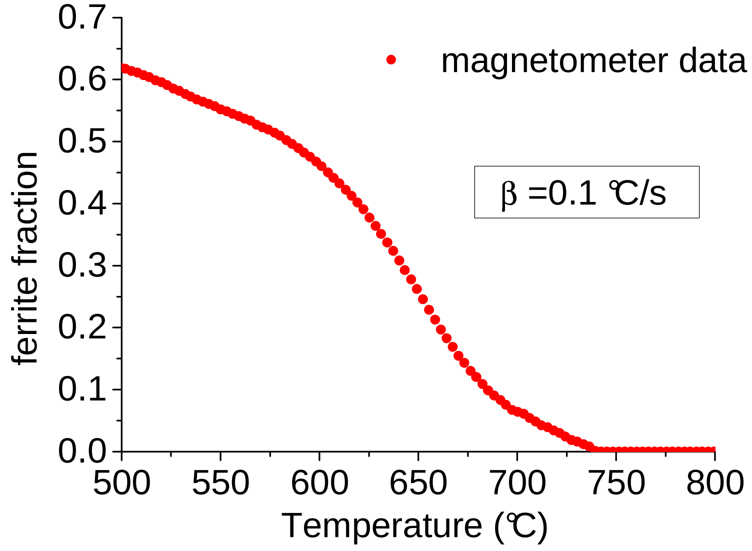
Fe - 0.16 C – 2.48 Mn – 2.96 Si (wt %)

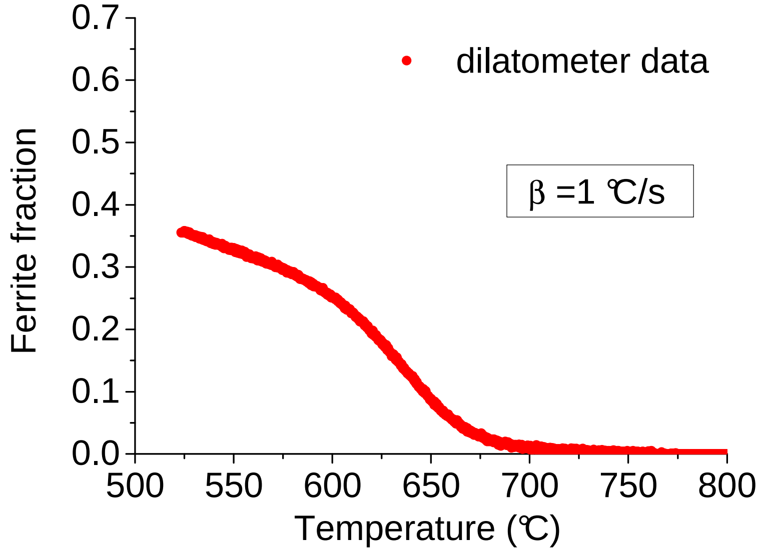






Experimental ferrite formation kinetics





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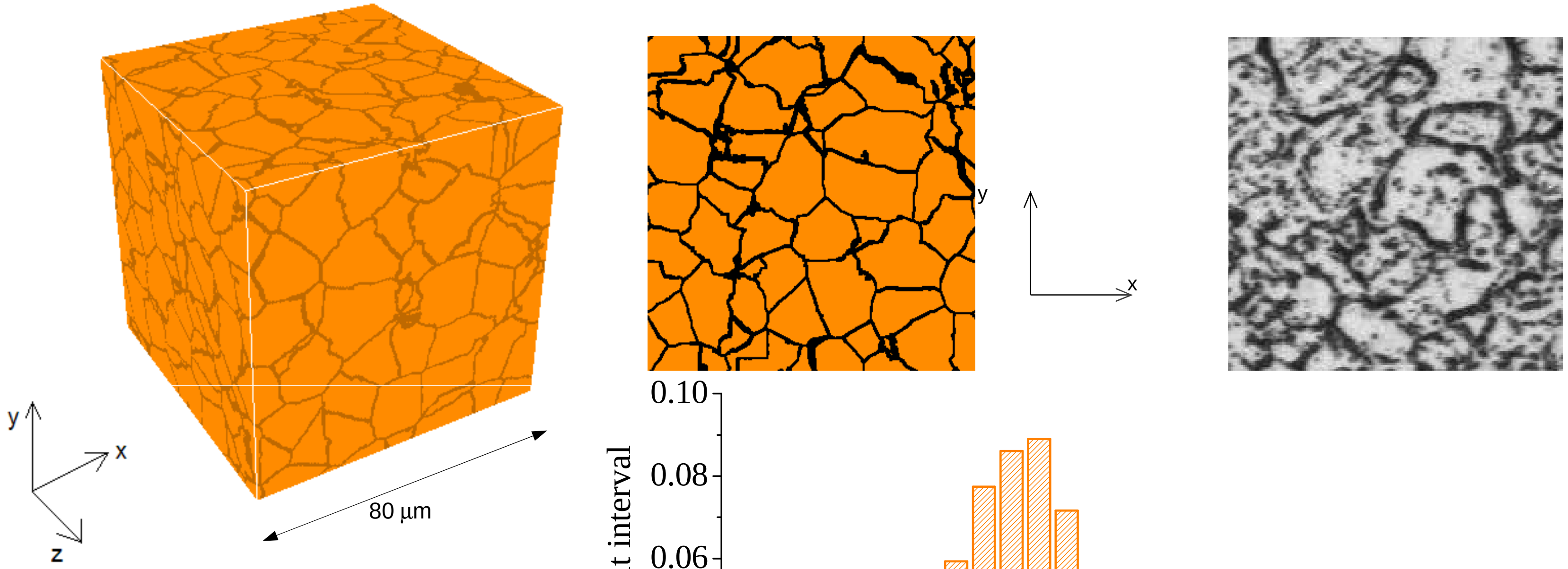
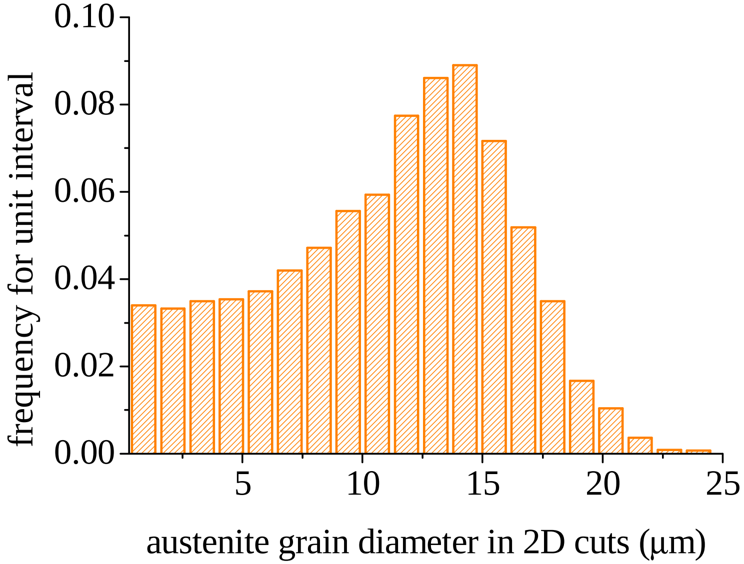
Input & output of the model

- Initial microstructure
- Composition and Mn profile
- Thermodynamic data
- Interface mobility & carbon diffusivity
- Parameters in nucleation rate equation

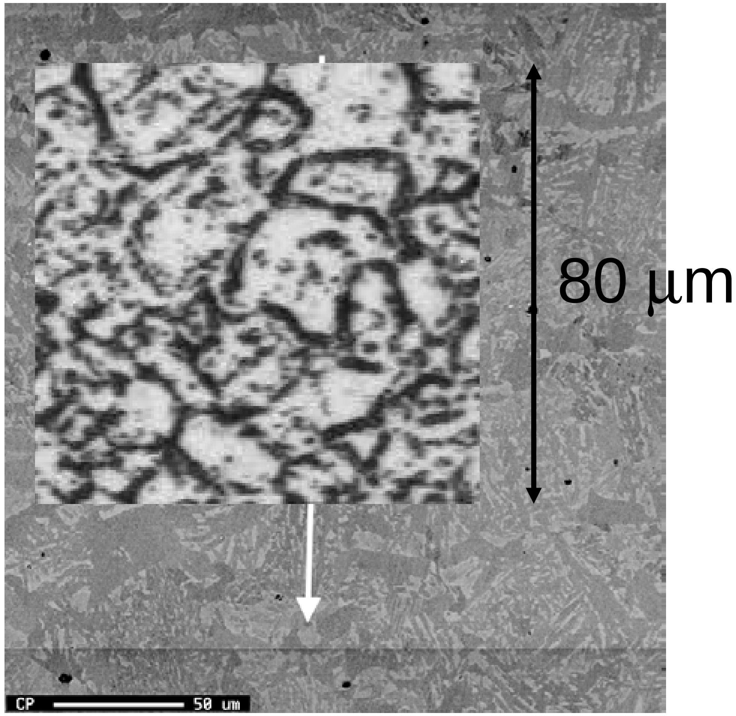
- Microstructure evolution
- C concentration at the interface and C concentration profile in γ

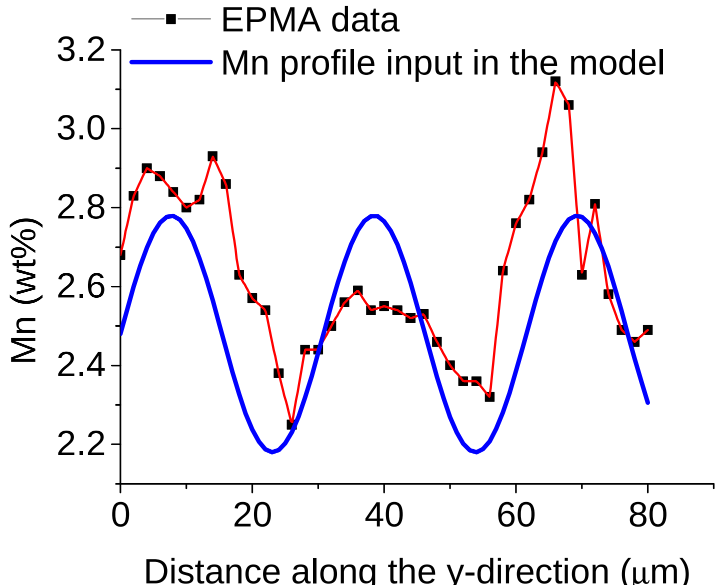
Input for 3D initial microstructure





Input of alloy element segregation





Validation of the model

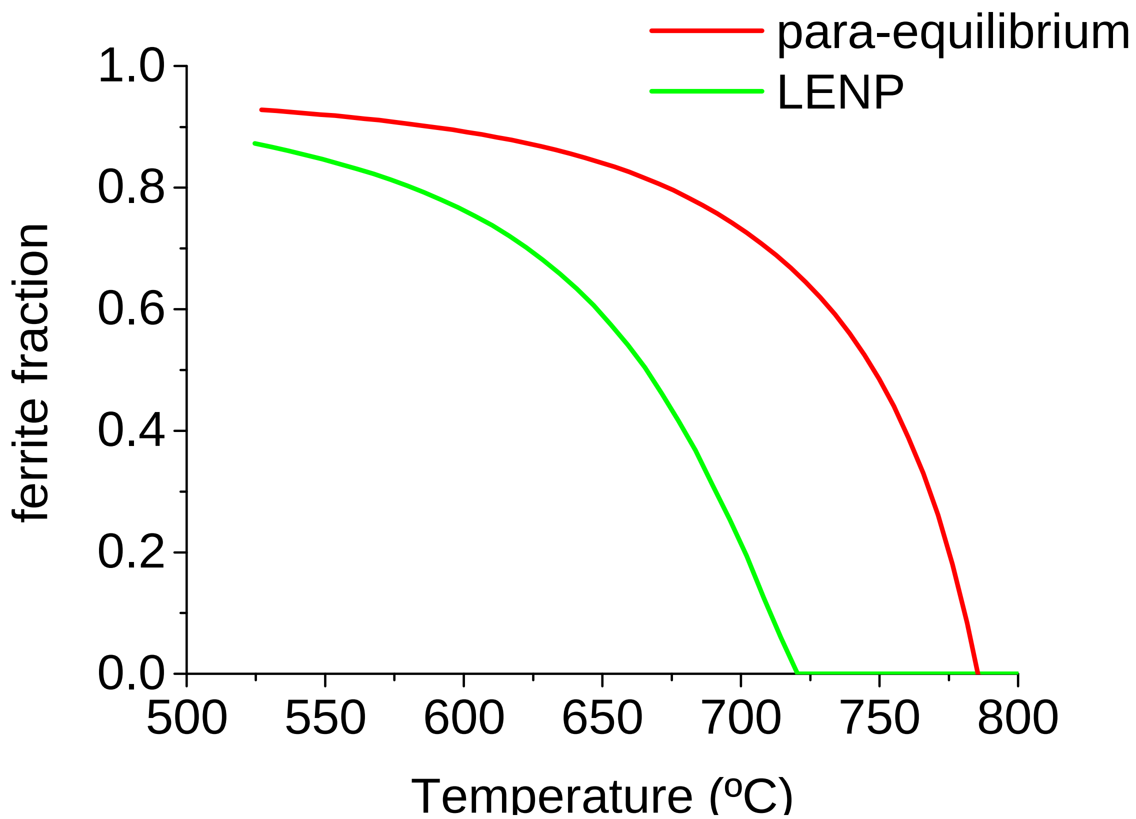
The ferrite fraction curves during cooling at 0.1 and 1 ºC/s cooling rate were used to validate the model

- The only adjusting parameter to fit the experimental ferrite fraction curves was the pre-exponential factor of the interface mobility.

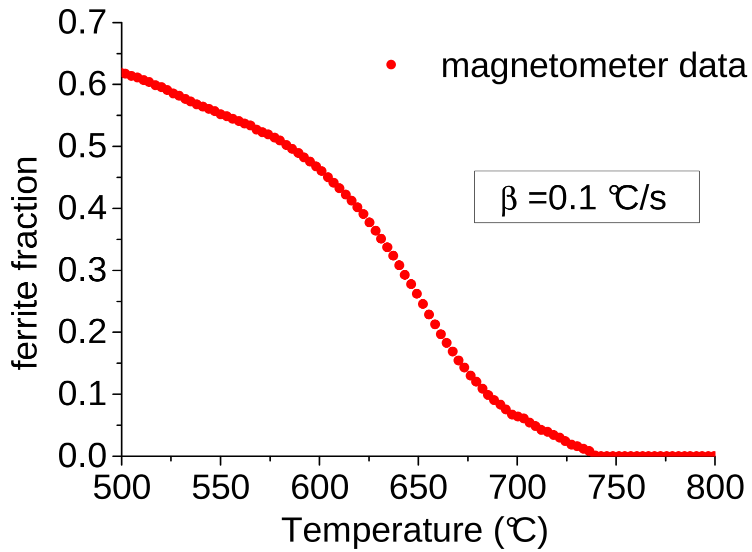
  $$M_{\alpha\gamma} = M_{\alpha\gamma}^{0} \exp\left(-140\ \text{kJ/mol} / RT\right)\ \text{m}^4\text{J}^{-1}\text{s}^{-1}$$

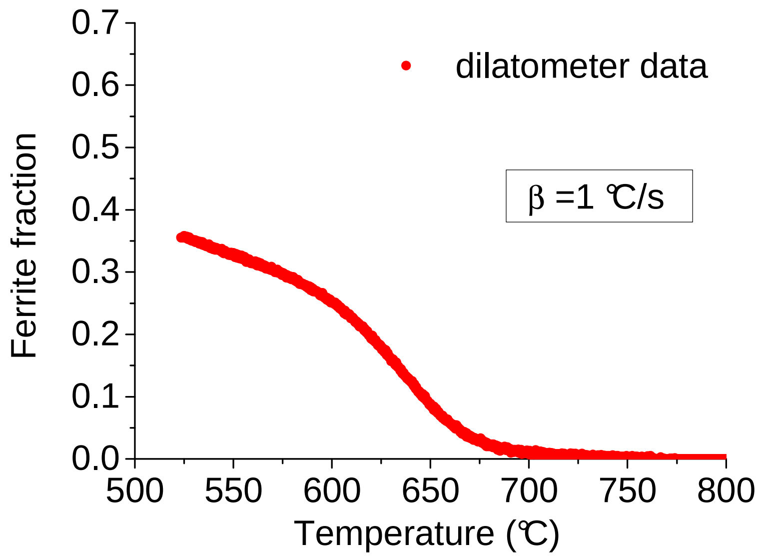
- The nucleation parameters (L & K_N) were selected to get experimental ferrite grain size in the microstructure after cooling

Thermodynamic condition at the interphase



Experimental ferrite formation kinetics





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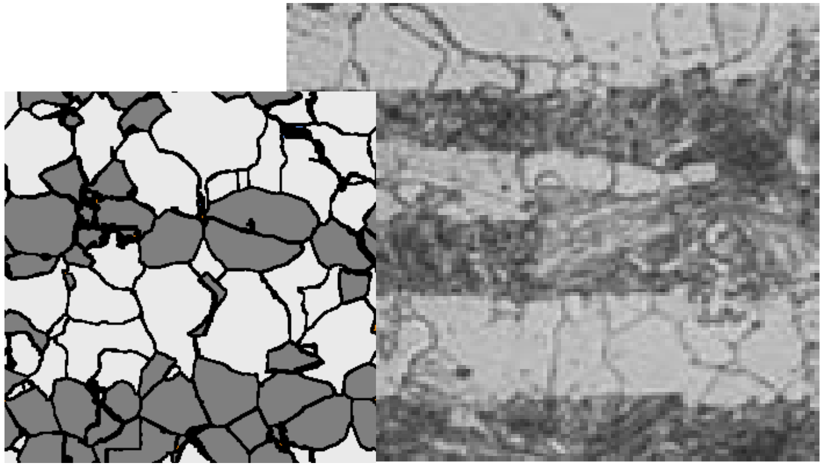
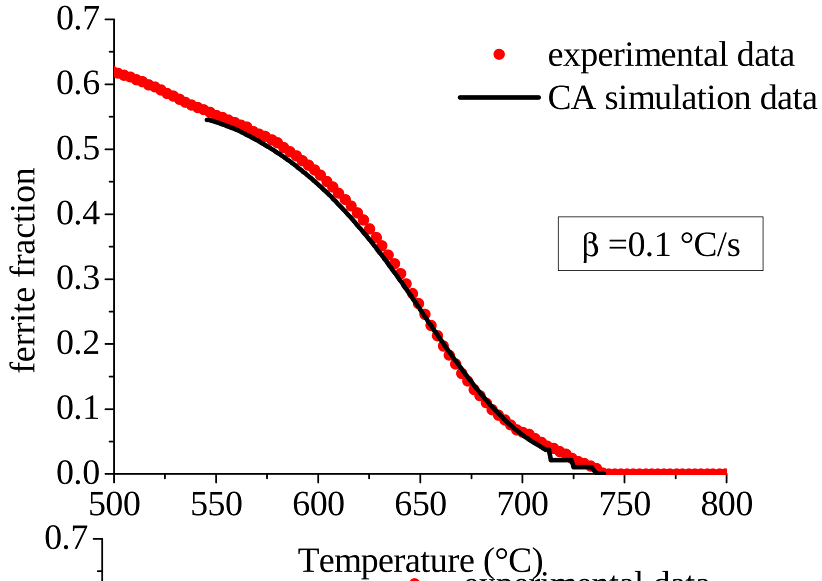
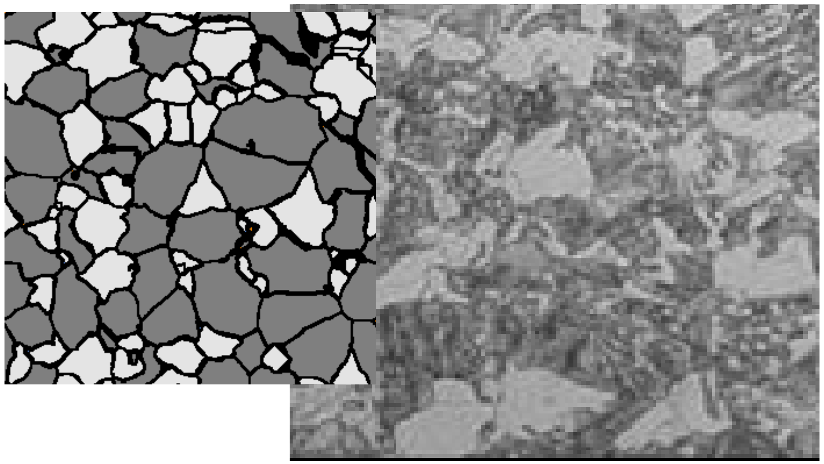
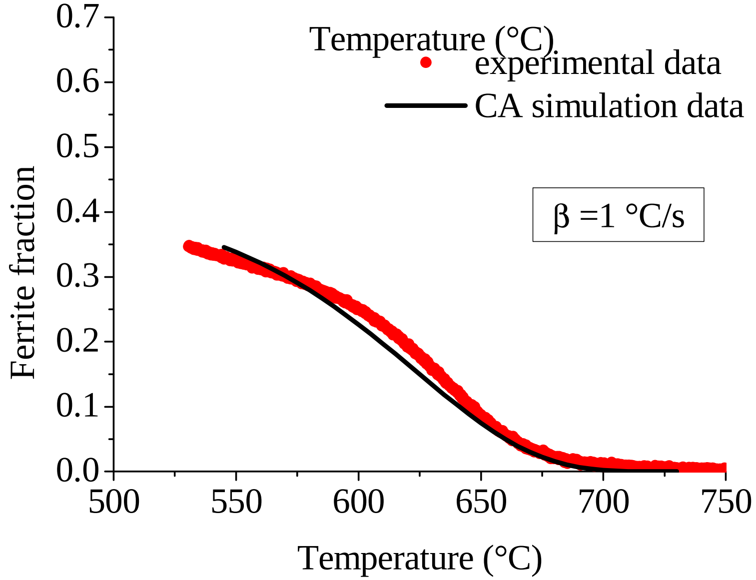
CA simulations at 0.1 and 1.0 °C/s







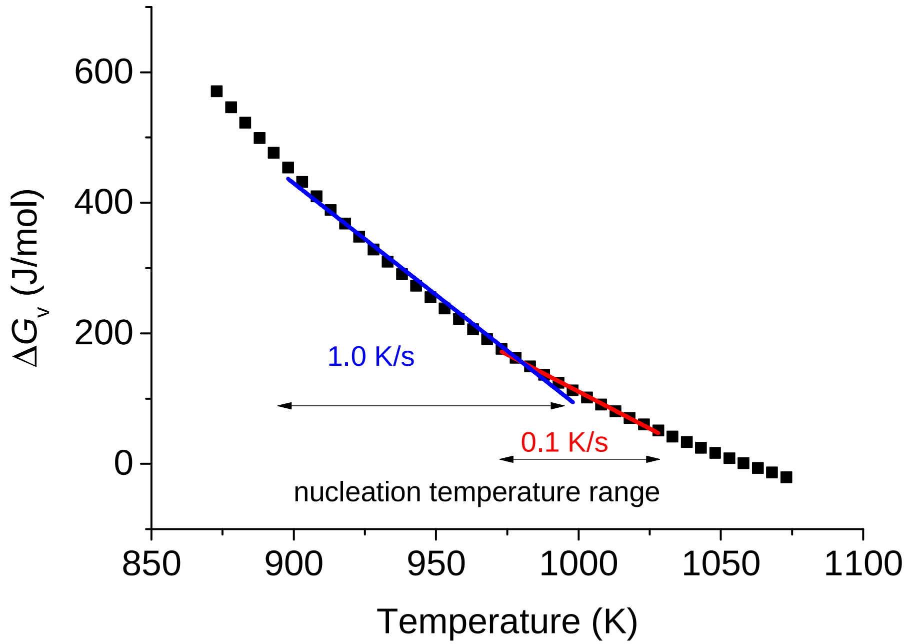


Best fitting parameters

	Growth		Nucleation		
β (K^{-1})	$M_0^{\alpha\gamma}$ $(\text{mol m J}^{-1}\ \text{s}^{-1})$	$Q_{\alpha\gamma}$ (kJ mol^{-1})	K_N	L (J K^{2})	Q_d (kJ mol^{-1})
0.1	0.006	140	1	2.5 x 10^{-16}	285
1.0	0.008				

CA model: best fitting parameters

$$L = \frac{\Psi}{\chi_T^{\;2}} = 2.5 \text{ x } 10^{-16} \text{ J K}^2 \text{ from the fitting}$$



$$\beta = 0.1 \text{ K/s}$$

$$\chi_T = 3.20 \text{ x } 10^5 \text{ J m}^{-3} \text{ K}$$

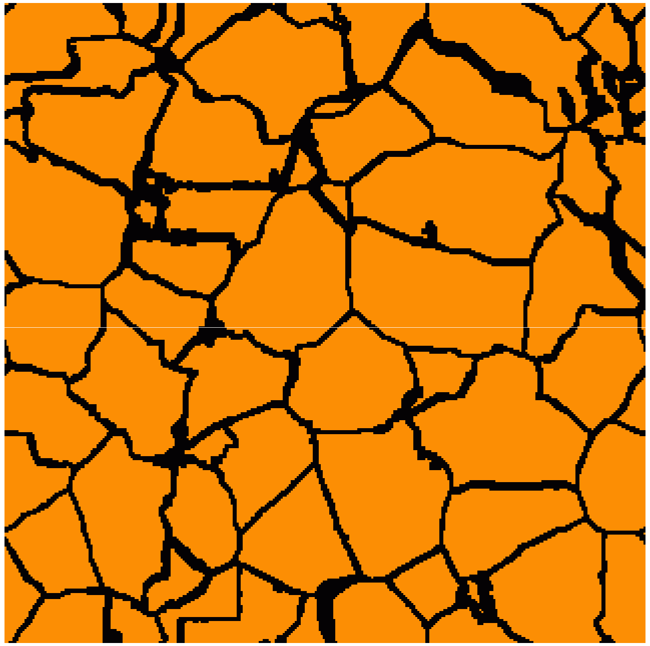
$$\Psi = 2.56 \text{ x } 10^{-5} \text{ J}^3 \text{ m}^{-6}$$

$$\beta = 1.0 \text{ K/s}$$

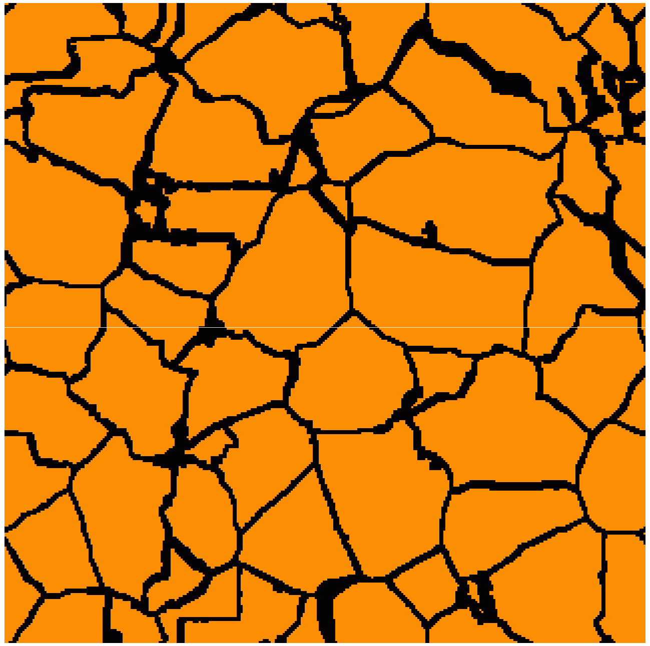
$$\chi_T = 4.82 \text{ x } 10^5 \text{ J m}^{-3} \text{ K}$$

$$\Psi = 5.82 \text{ x } 10^{-5} \text{ J}^3 \text{ m}^{-6}$$

Microstructure during cooling



$\beta = 0.1\ ^oC/s$



$\beta = 1.0\ ^oC/s$

Conclusion

- A very good agreement between the simulated and experimental ferrite fraction curve is obtained over the entire temperature range for ferrite formation, if the transition from PE to LENP conditions at the interface is assumed to occur just after ferrite nucleation.

- The microstructural banding is excellently reproduced in the simulated microstructure.

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