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The cyclic phase transformation concept and the effective interface mobility

E. Gamsjäger[1], Hao Chen[2], Sybrand van der Zwaag[2]

[1]Montanuniversität Leoben, Institute of Mechanics, Leoben, Austria.
[2]Faculty of Aerospace Engineering, Delft University of Technology, The Netherlands.

Contents

- **Motivation**
  - ➢ Diffusive phase transformations

    (e.g. solid / liquid or solid/solid phase transformations)

- **Model 1 (LE)**
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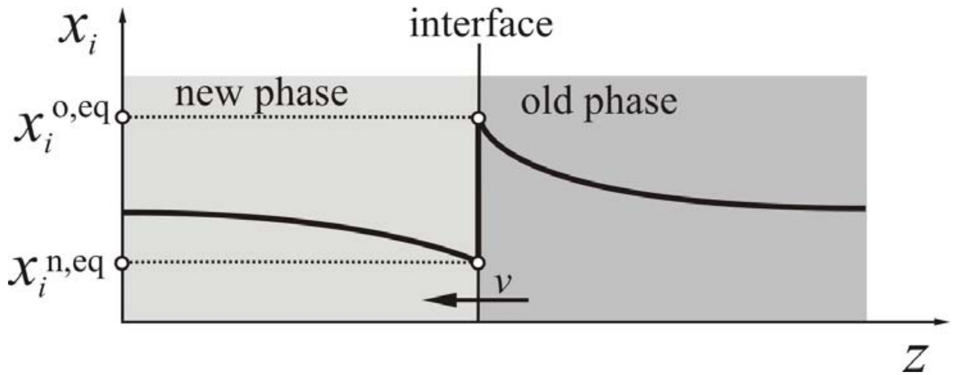
- **Model 2 (thick interface) / Model 3 (effective interface mobility)**
  - ➢ Theory and modeling results

- **Model 1 / Model 3**
  - ➢ Cyclic phase transformations

- **Conclusions and Outlook**

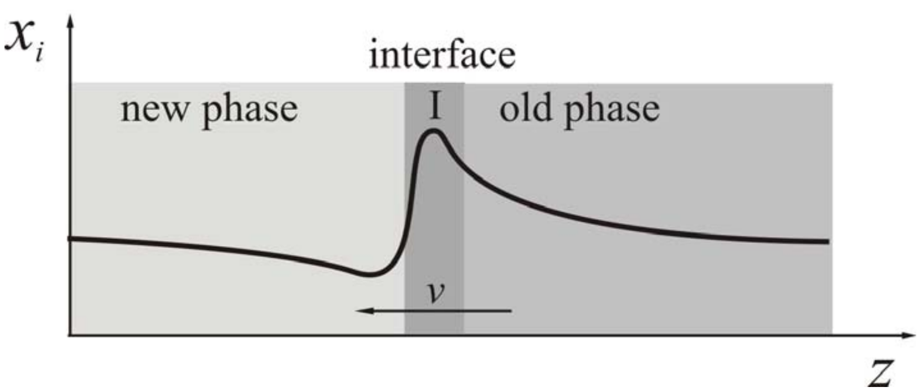
Theory

Model 1: Sharp interface, infinite mobility **LE(NP)**

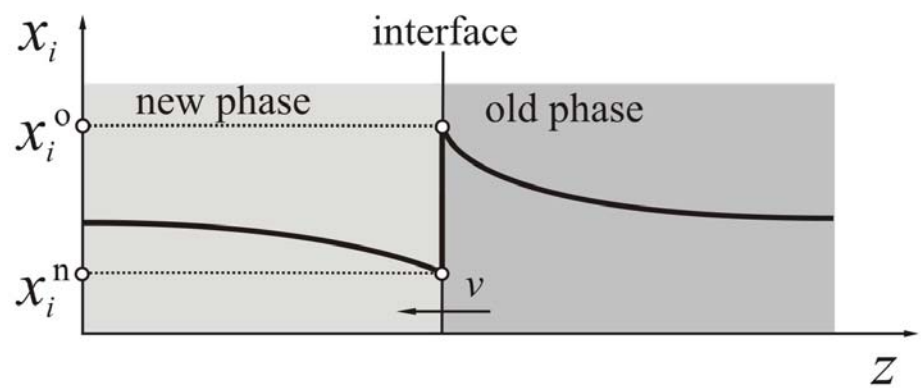


~~$v = M\Delta f$~~

Model 2: Interfacial region
(Thick interface)



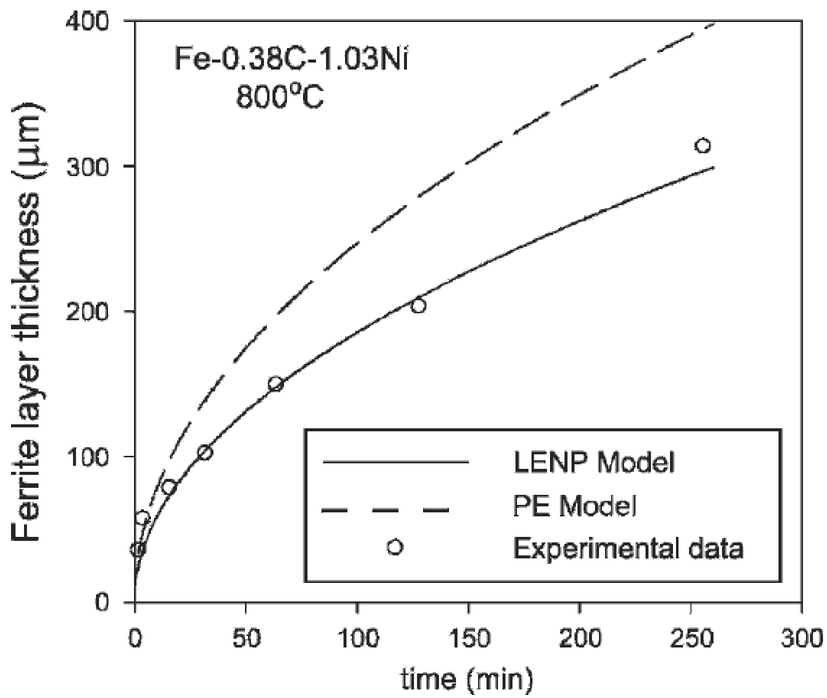
Model 3: Finite mobility (SI):
(Effective interface mobility, no substitutional bulk diffusion)

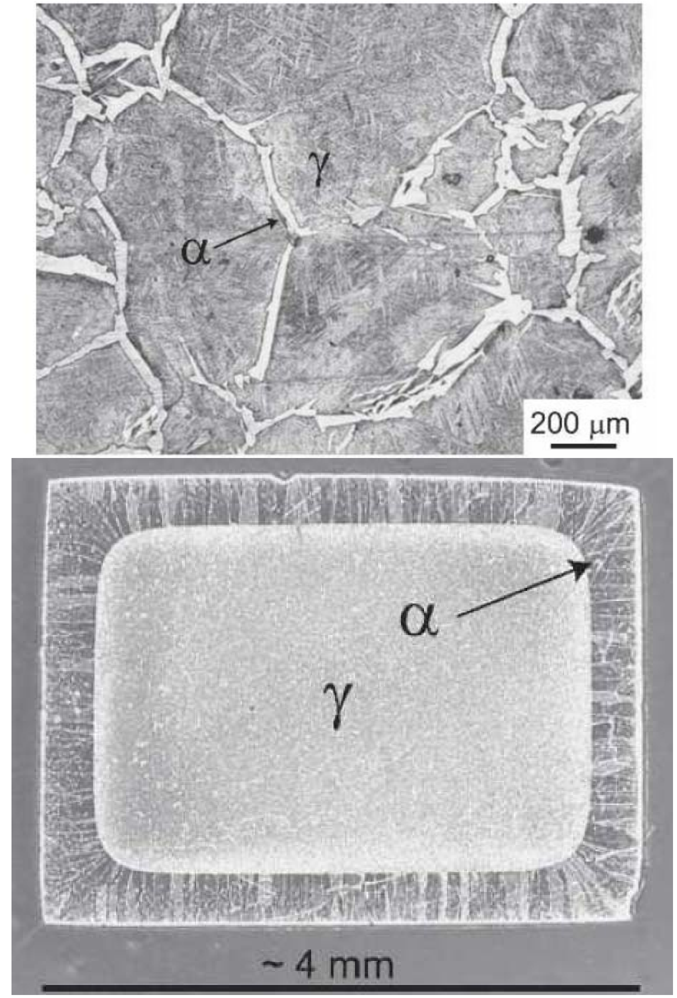


$$v = M\Delta f$$

Model 1: Sharp interface, infinite mobility **LE(NP)**

$\gamma \rightarrow \alpha$ transformation: Fe-C-Ni

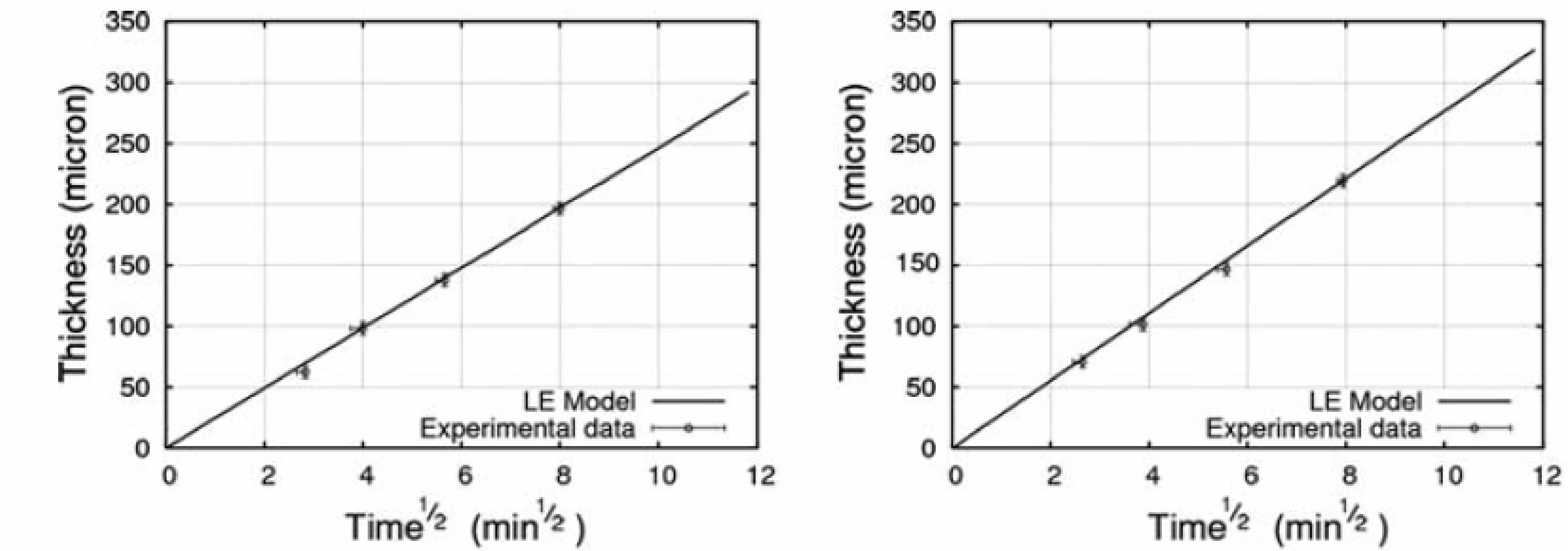




From: C. R. Hutchinson, H. S. Zurob, Y. Bréchet: Metall. Mater. Trans. (37A) 2006, 1711-1720.

Model 1: Sharp interface, infinite mobility **LE(NP)**

$\gamma \rightarrow \alpha$ transformation: Fe-C

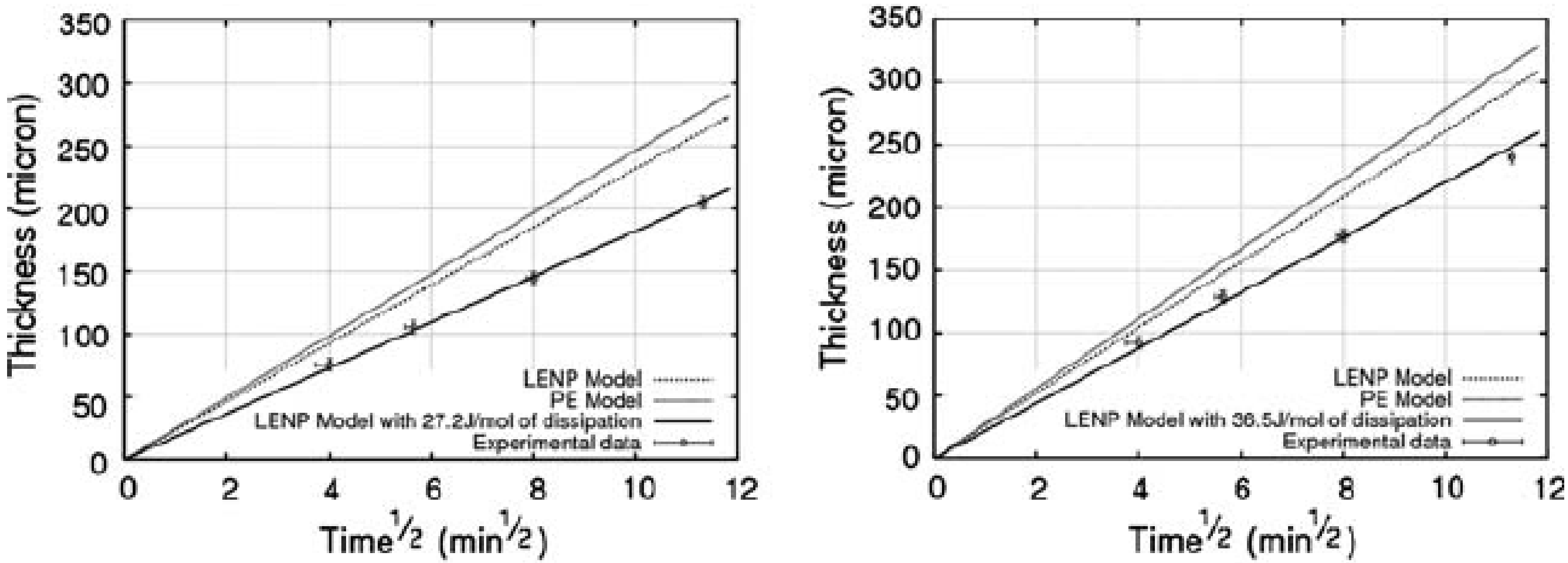


Ferrite layer growth kinetics during decarburization of an Fe-0.57C (mass frac. in %) binary alloy at 850°C and 825°C.

From: A. Béché, H. S. Zurob, C. R. Hutchinson: Metall. Mater. Trans. (38A) 2007, 2950-2955.

Model 1: Sharp interface, infinite mobility **LE(NP)**

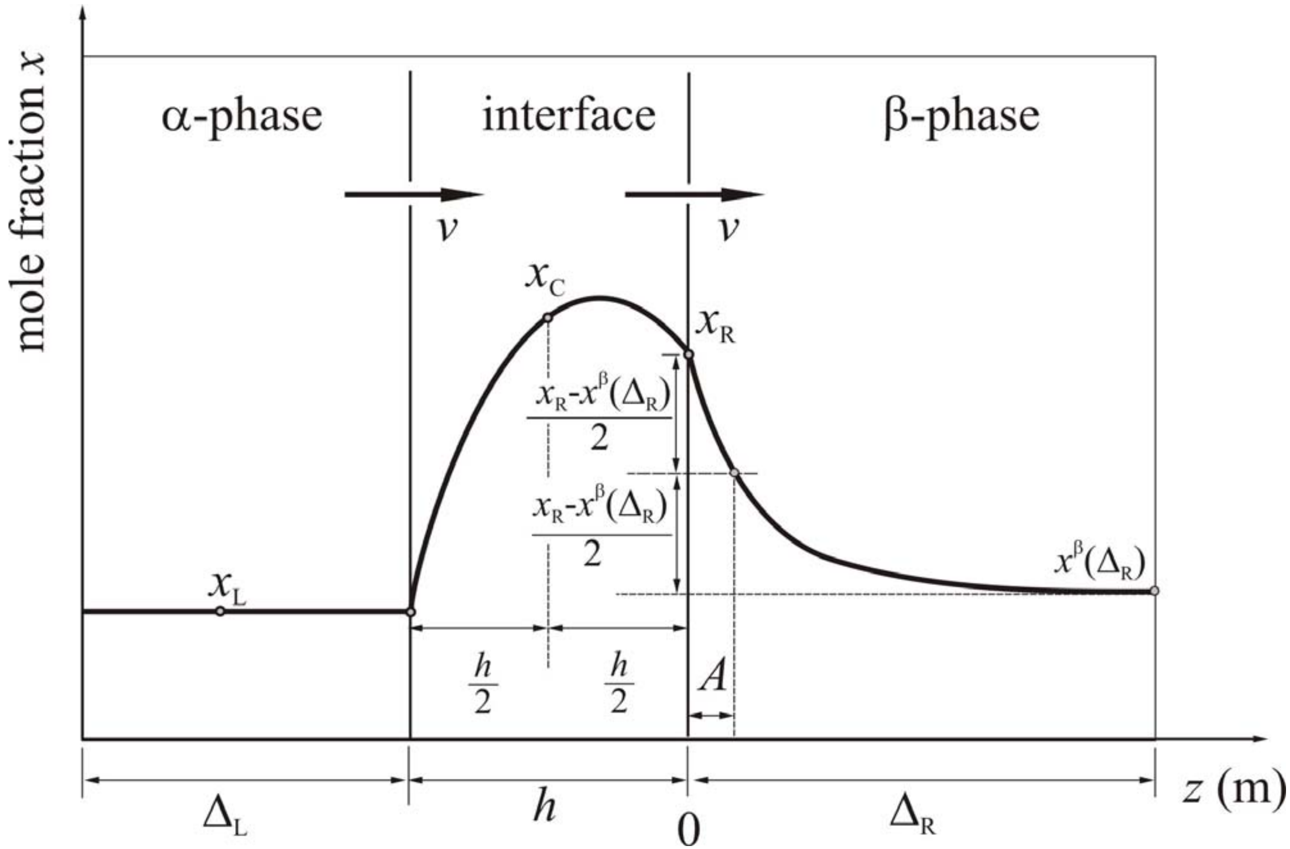
$\gamma \rightarrow \alpha$ transformation: Fe-C-Cr



Ferrite layer growth kinetics during decarburization of an Fe-0.58C-2.0Cr (mass frac. in %) alloy at 806°C and 775°C.

From: A. Béché, H. S. Zurob, C. R. Hutchinson: Metall. Mater. Trans. (38A) 2007, 2950-2955.

Model 2: Thick interface parametric model

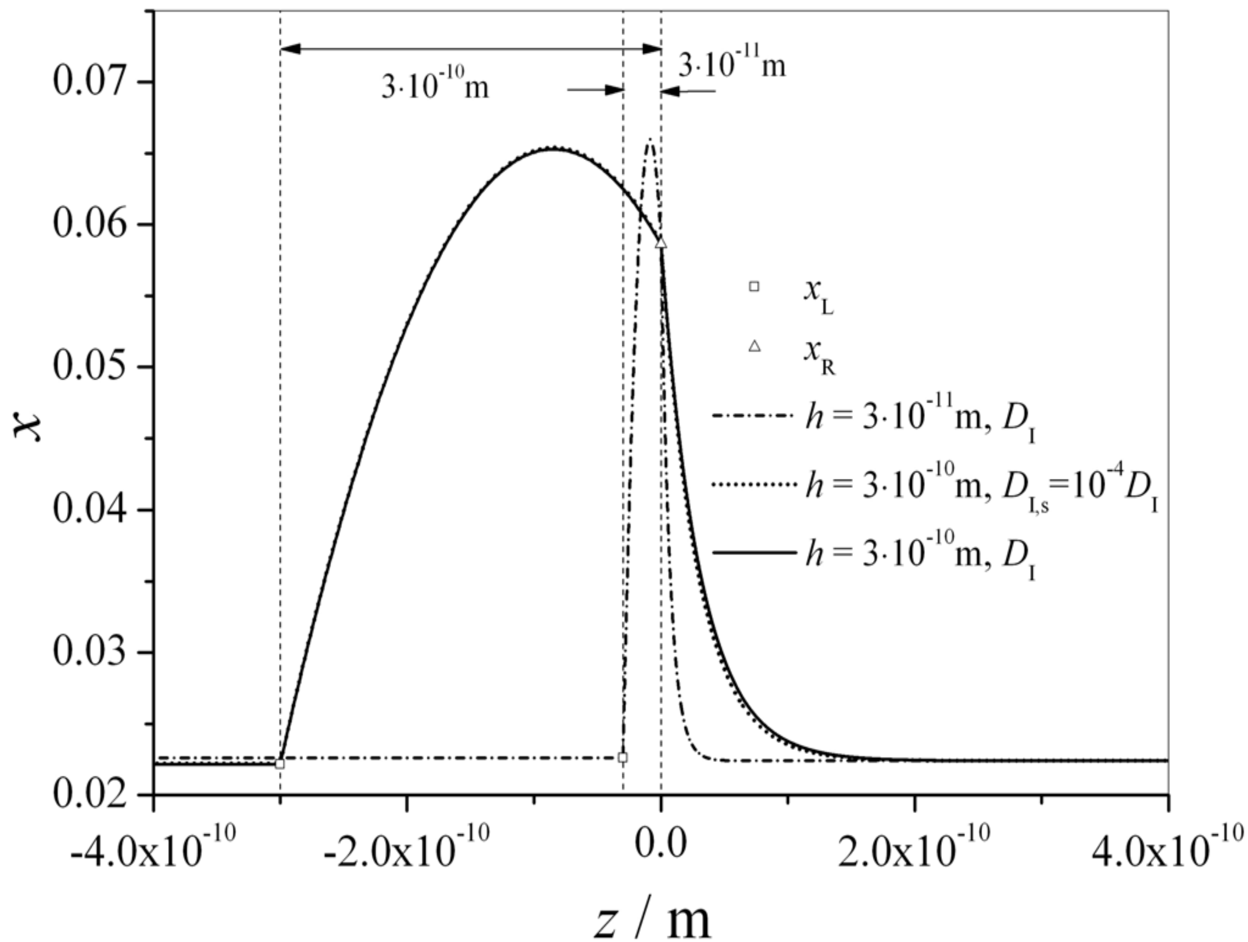


$$x^{\mathrm{int}}(z) = 2(x_L - 2x_C + x_R)\left(\frac{z}{h}\right)^2 + (x_L - 4x_C + 3x_R)\left(\frac{z}{h}\right) + x_R$$

$$x^\beta(z) = B\left(\exp\left(-\frac{z}{A}\right) + \exp\left(-\frac{2\Delta_R - z}{A}\right)\right) + x^\beta_{\mathrm{start}}$$

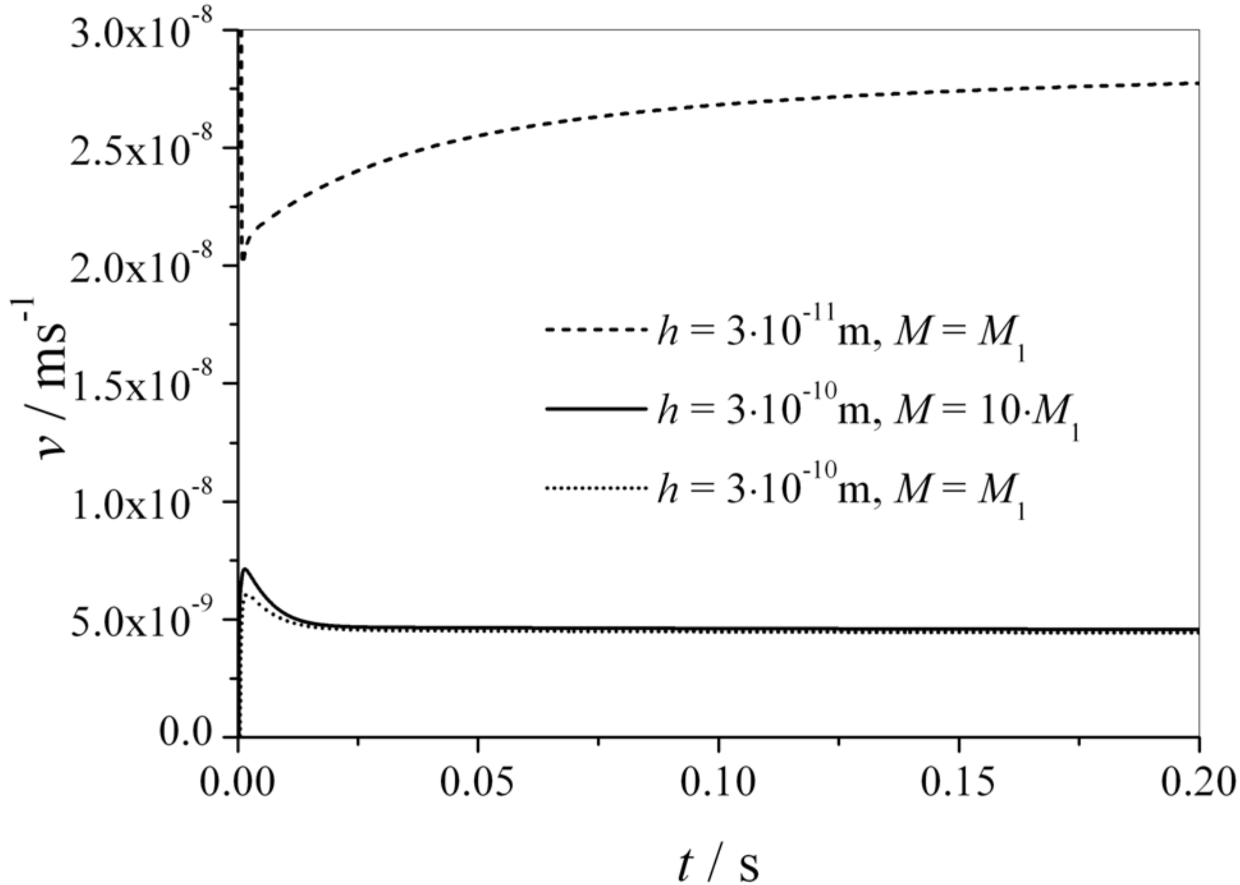
J. Svoboda, E. Gamsjäger: "Modelling of diffusive and massive phase transformations in binary systems – thick interface parametric model", *Int. J. Mater. Res.* **102** (2011) 666-673.

Model 2: Fe-Mn system

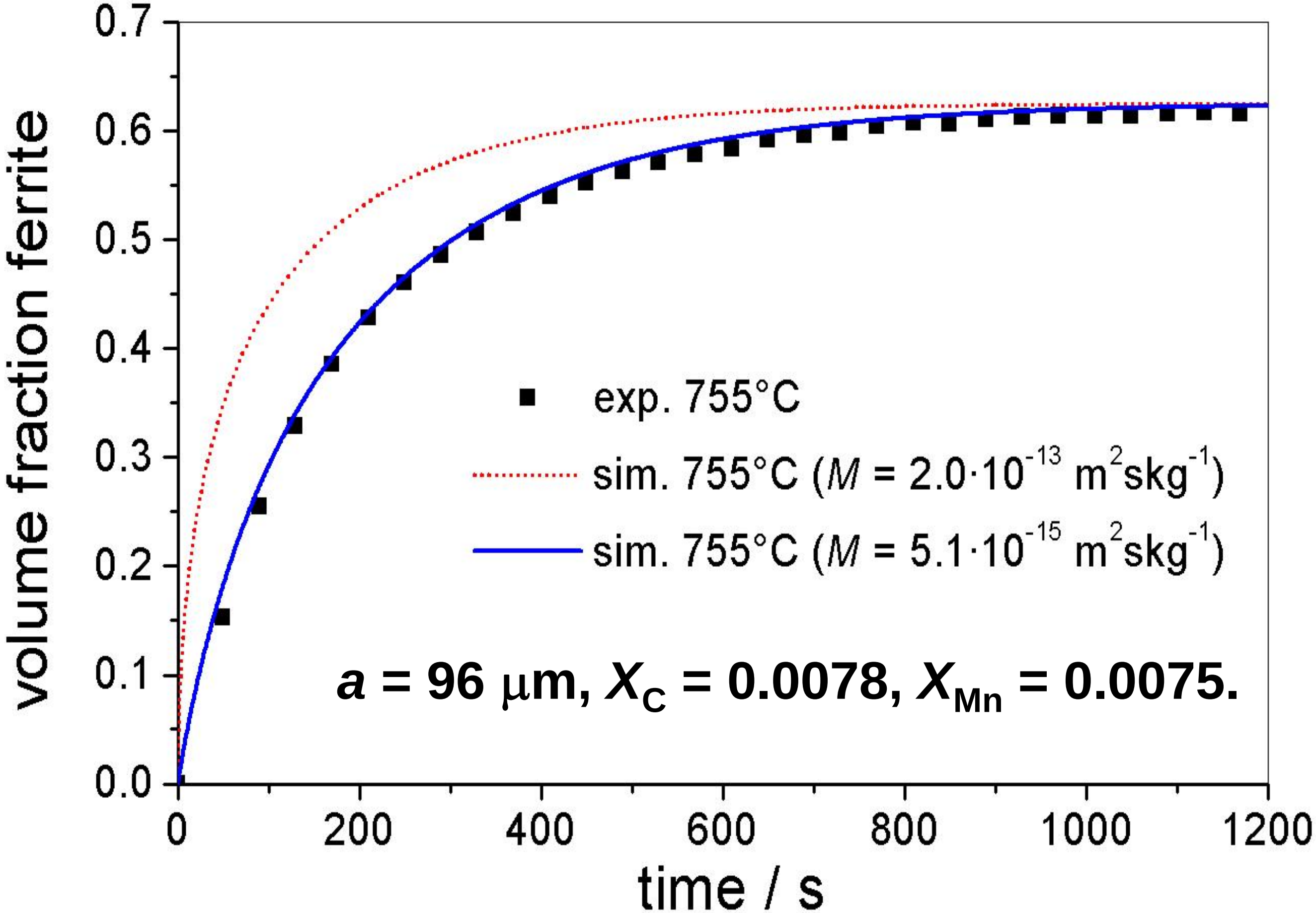


E. Gamsjäger, R.E. Werner, W. Schiller, B. Buchmayr, Steel Res. Int. (2013), in press.

Model 2: Fe-Mn system

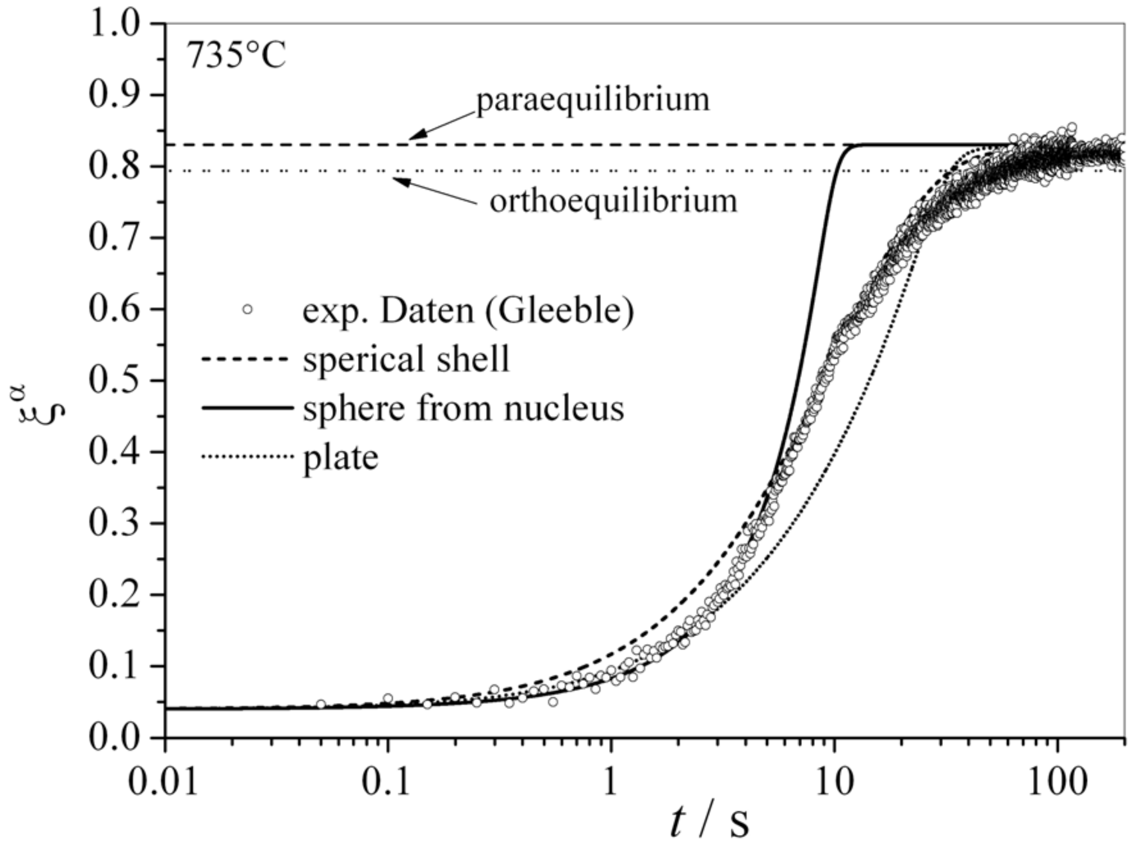


Model 3: Fe-Mn-C system



E. Gamsjäger, J. Svoboda, F.D. Fischer: "Austenite-to-ferrite phase in low-alloyed steels", *Comput. Mater. Sci.* **32** (2005) 360-369.

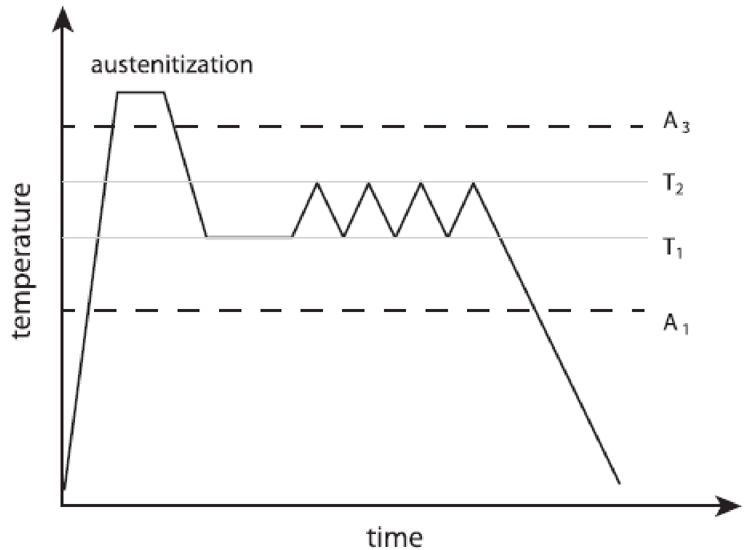
Model 3: (Fe-C-Mn-Si)



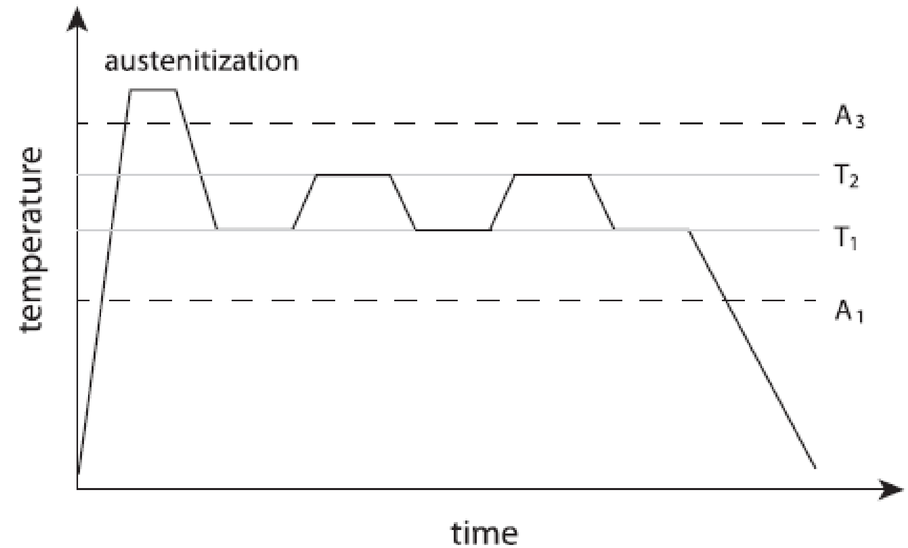
E. Gamsjäger, R.E. Werner, W. Schiller, B. Buchmayr : Steel Res. Int. (2013) in press.

Novel experimental approach:
Cyclic phase transformations

I-type exeriment



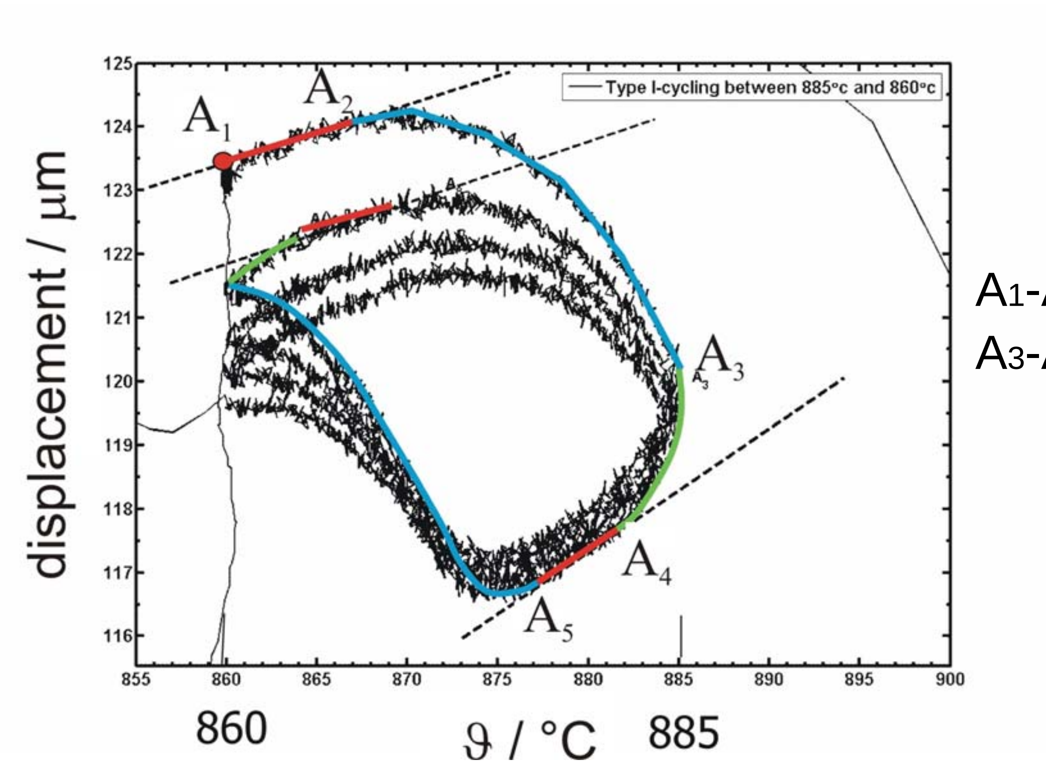
H-type exeriment



H. Chen, B. Appolaire, S. van der Zwaag : Acta Mater. 59 (2011) 6751-6760.

Novel experimental approach:
Cyclic phase transformations

I-type exeriment

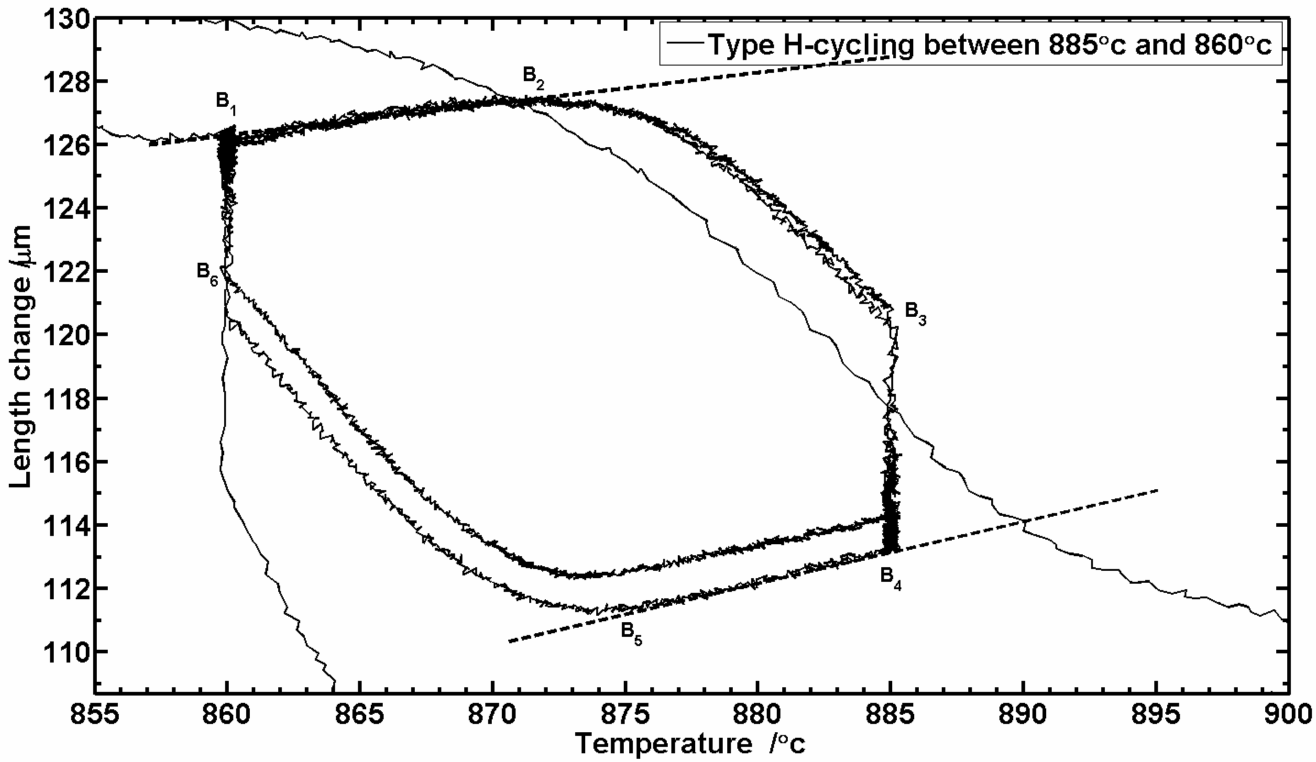


A_1-A_2 and A_4-A_5: stagnant stage

A_3-A_4: Inverse phase transformation

H. Chen, B. Appolaire, S. van der Zwaag : Acta Mater. 59 (2011) 6751-6760.

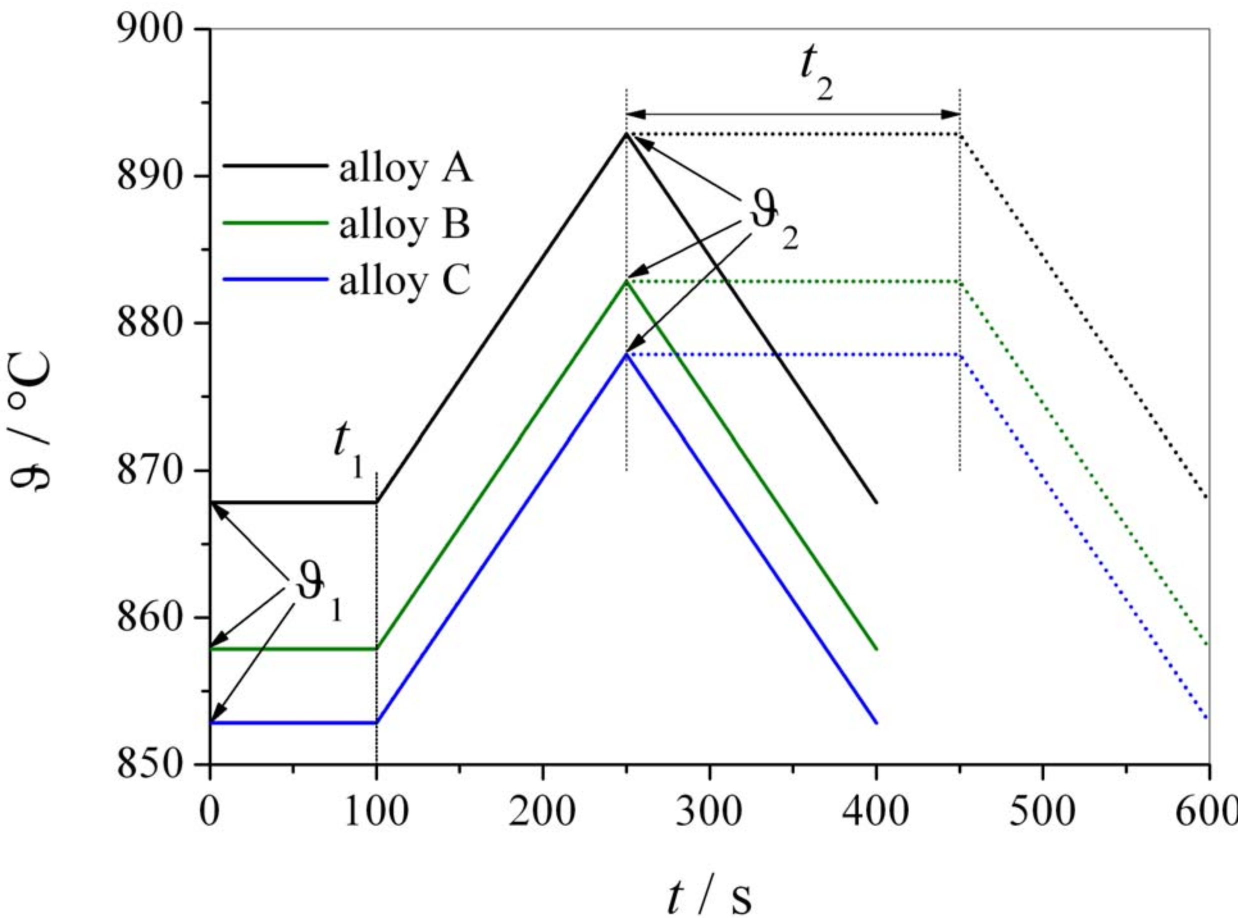
Novel experimental approach:
Cyclic phase transformations



B_1-B_2 and B_4-B_5: stagnant stage

H. Chen, B. Appolaire, S. van der Zwaag : Acta Mater. 59 (2011) 6751-6760.

Heat treatment in the computer simulations



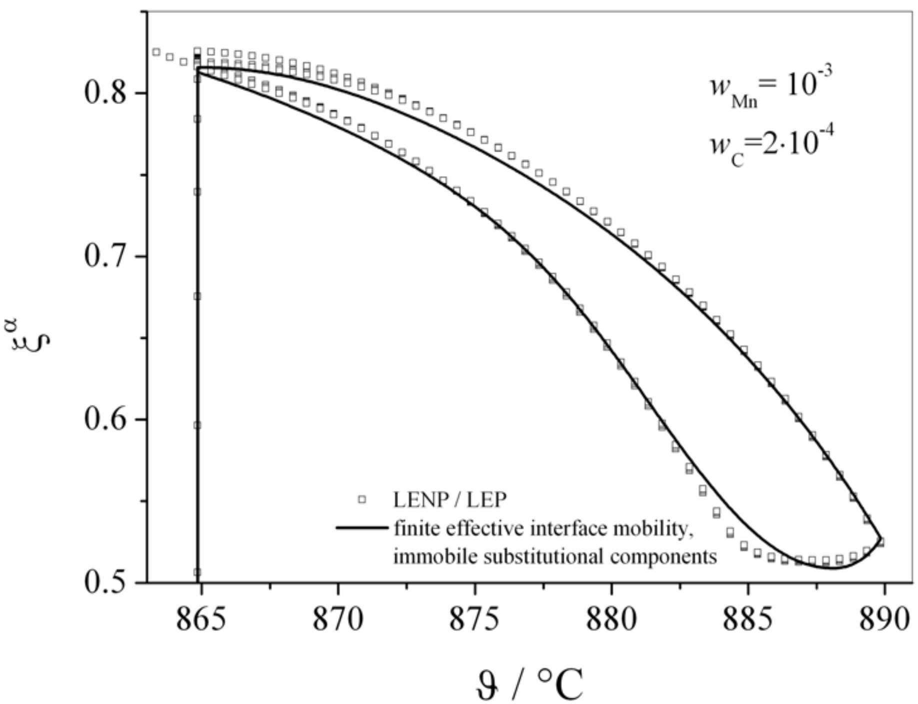
Alloy A: $w_{Mn} = 1 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$

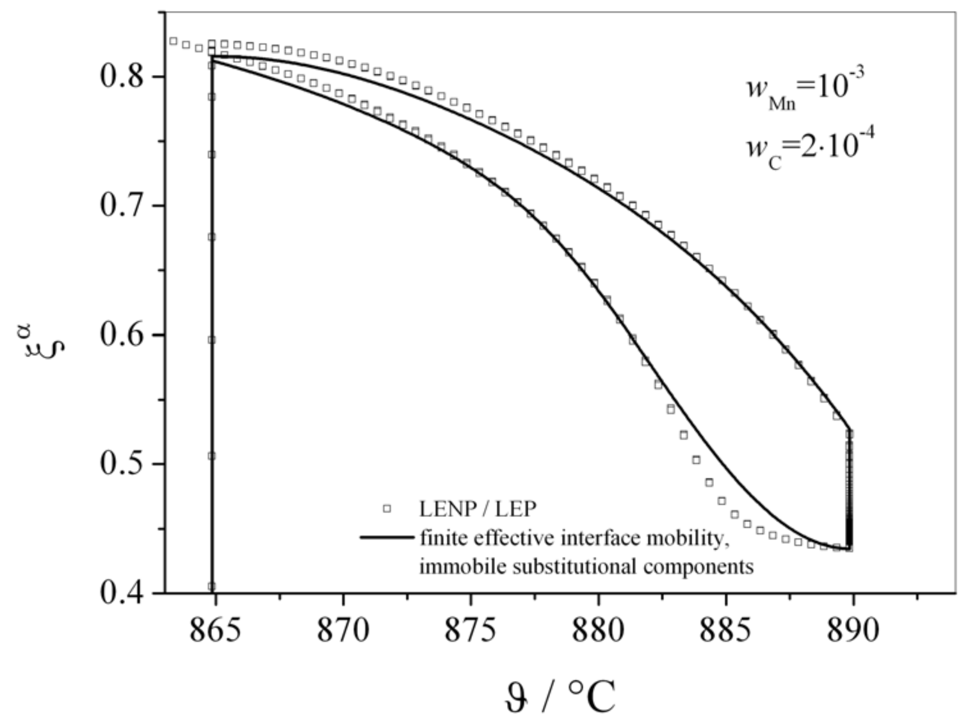
Alloy B: $w_{Mn} = 2 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$

Alloy C: $w_{Mn} = 3 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$

Comparison of Model 1 and Model 3

Alloy A:



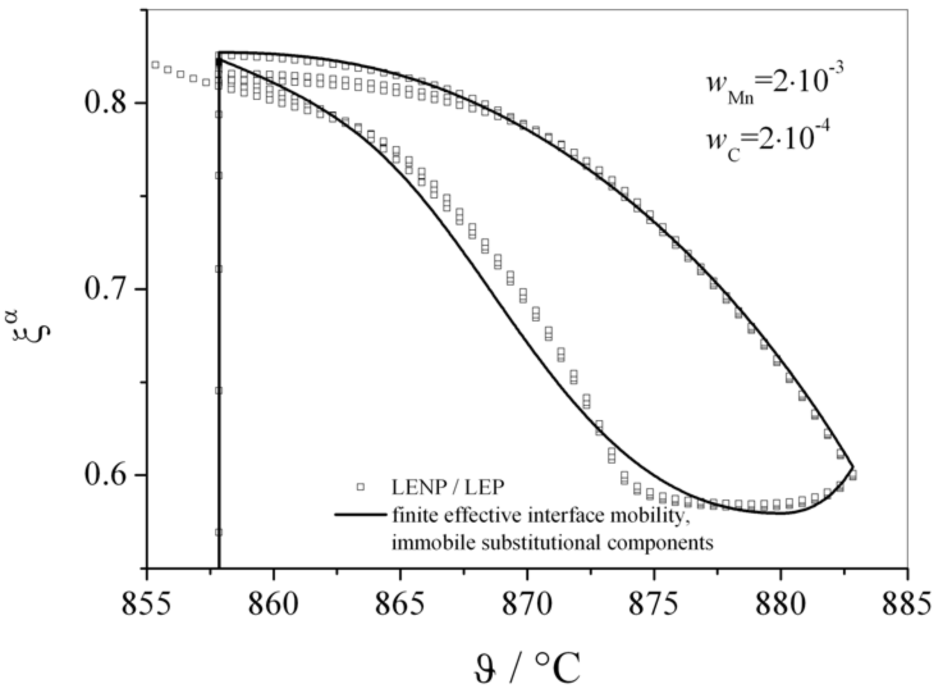


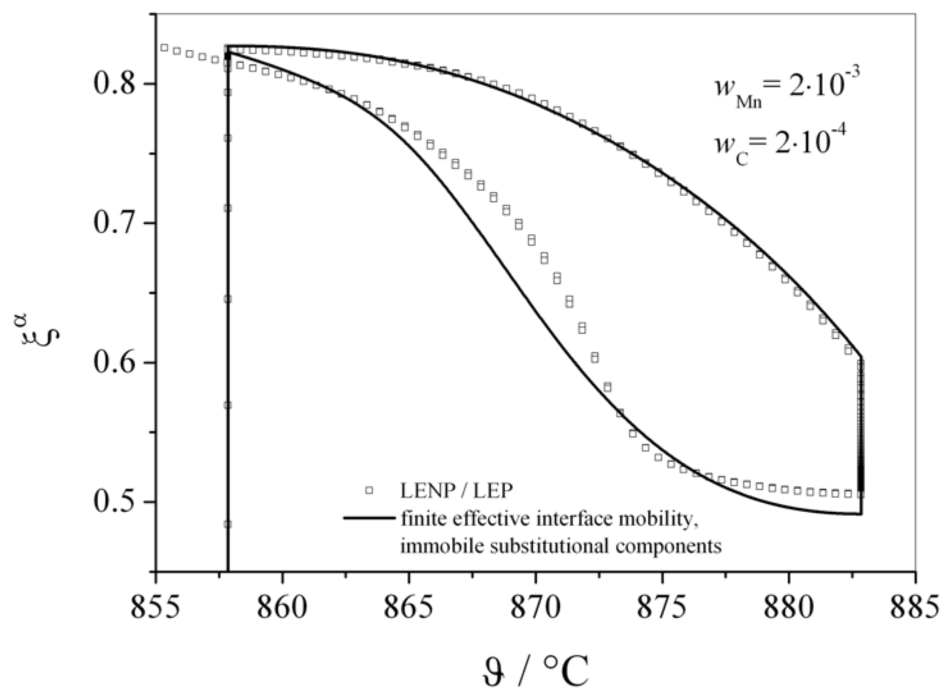
□ local equilibrium; —— effective mobility

E. Gamsjäger, H. Chen, S. van der Zwaag: in preparation.

Comparison of Model 1 and Model 3

Alloy B:



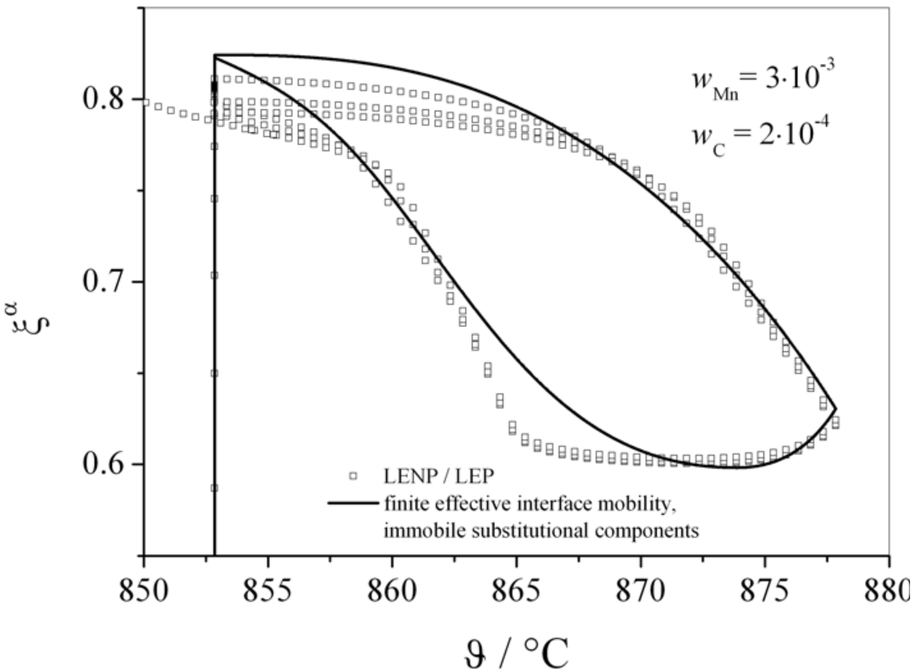


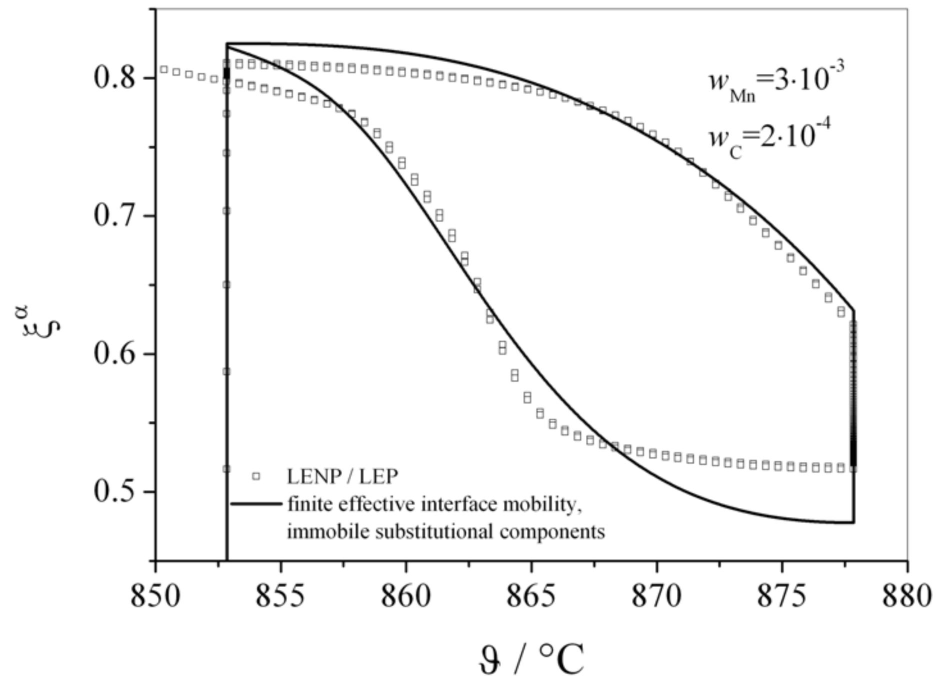
□ local equilibrium; ——— effective mobility

E. Gamsjäger, H. Chen, S. van der Zwaag: in preparation.

Comparison of Model 1 and Model 3

<u>Alloy C:</u>



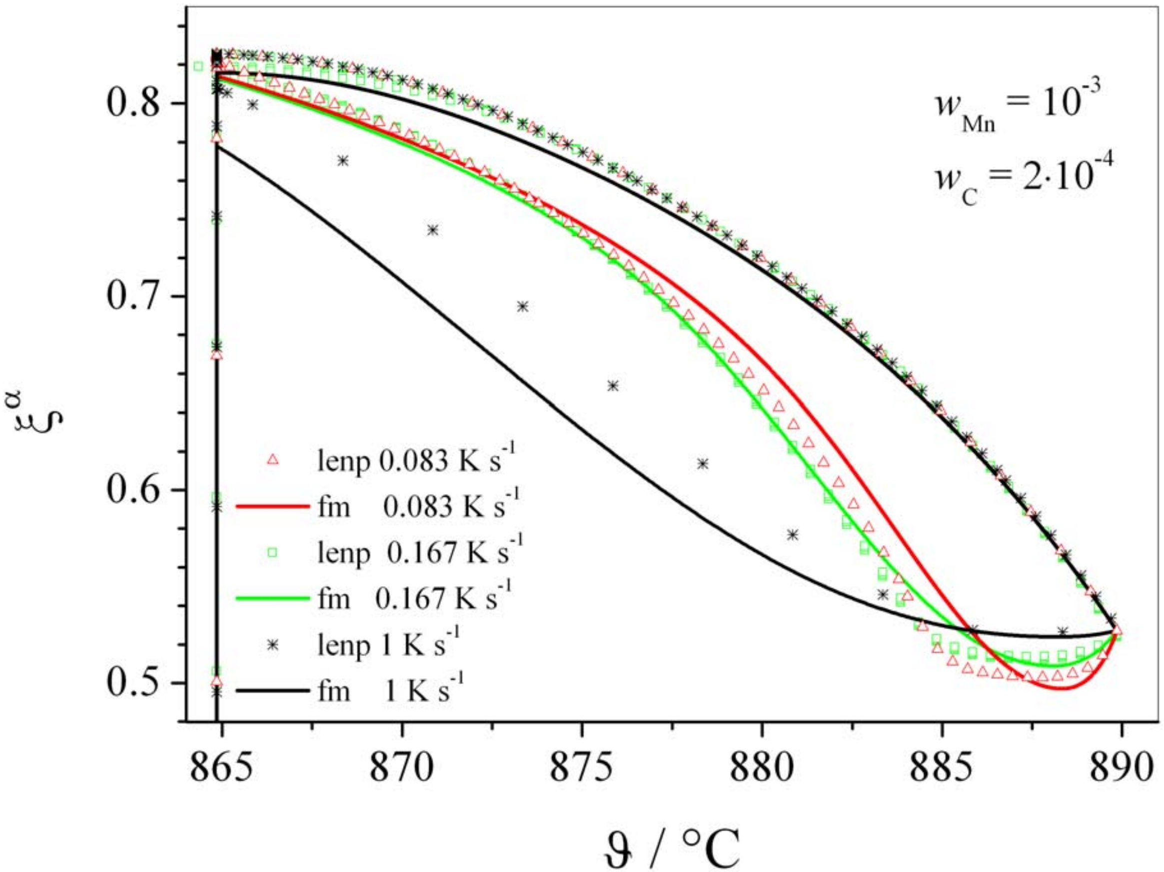


□ local equilibrium; ——— effective mobility

E. Gamsjäger, H. Chen, S. van der Zwaag: in preparation.

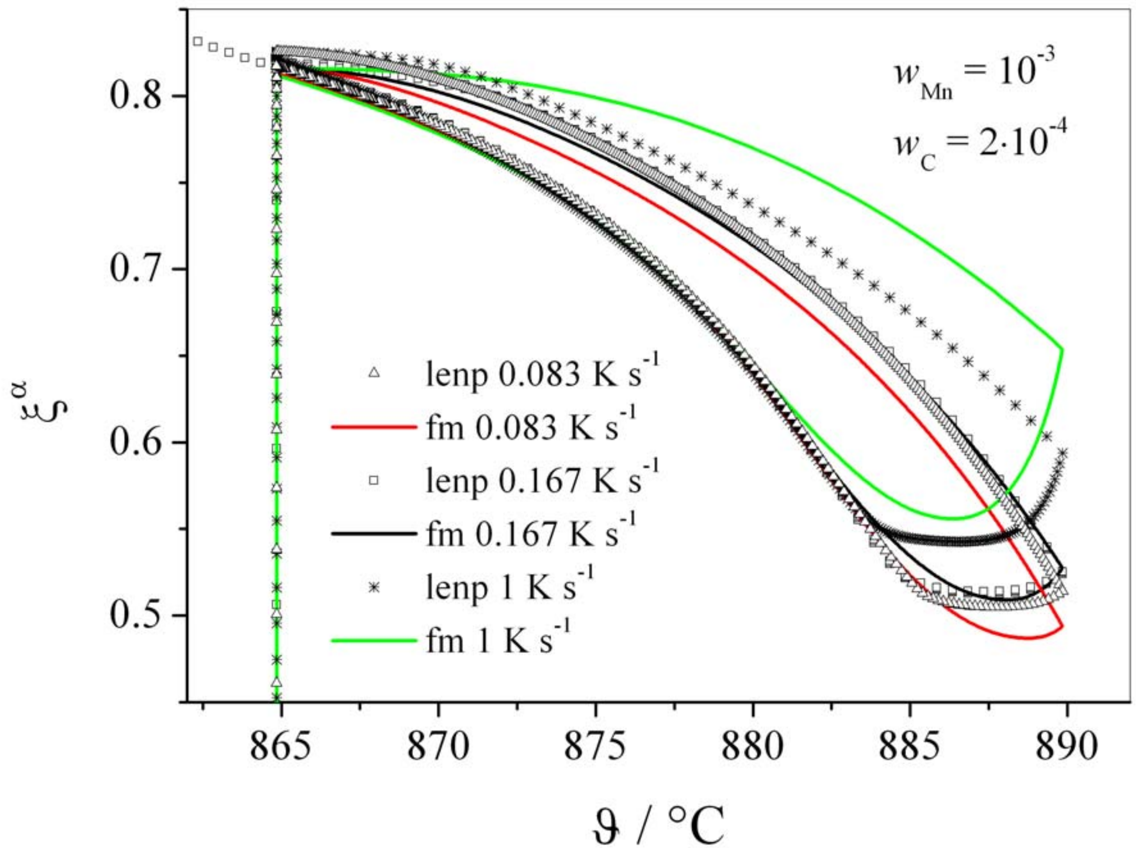
Comparison of Model 1 and Model 3

Different cooling rates:



Comparison of Model 1 and Model 3

Different heating rates:



Effective mobility

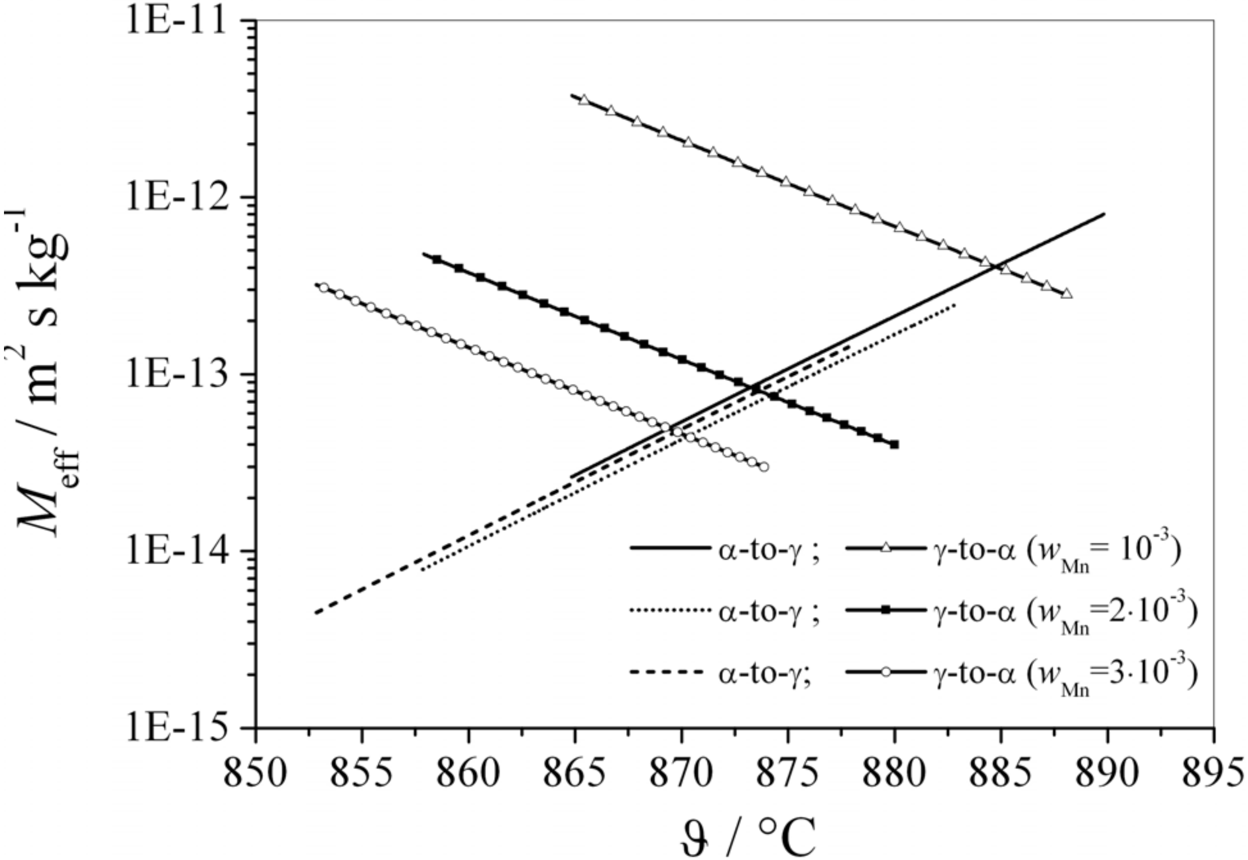
$$M_{\text{eff}} = M_0 \cdot \exp\left[\frac{1}{RT}\left(-Q + a(T - T_{\text{S}})\right)\right]$$

$$Q = 140 \cdot 10^3 \text{ J mol}^{-1} \text{ K}^{-1}$$

Table 1: Coefficients for the different model alloys

	ϑ - range	T_S / K	M_0 / m^2 s kg^{-1}	a / J mol^{-1} K^{-1}	Composition
$\alpha \rightarrow \gamma$	$864.85°C \le \vartheta$ $\vartheta \le 889.85°C$	1138	$7 \cdot 10^{-8}$	$1.2 \cdot 10^3$	$w_{Mn} = 10^{-3}$; $w_C = 2 \cdot 10^{-4}$
$\gamma \rightarrow \alpha$	$864.85°C \le \vartheta$ $\vartheta \le 889.85°C$	1138	$1 \cdot 10^{-5}$	$-1.2 \cdot 10^3$	$w_{Mn} = 10^{-3}$; $w_C = 2 \cdot 10^{-4}$
$\alpha \rightarrow \gamma$	$857.85°C \le \vartheta$ $\vartheta \le 882.85°C$	1131	$2.3 \cdot 10^{-8}$	$1.2 \cdot 10^3$	$w_{Mn} = 2 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$
$\gamma \rightarrow \alpha$	$857.85°C \le \vartheta$ $\vartheta \le 882.85°C$	1131	$1.4 \cdot 10^{-6}$	$-1.2 \cdot 10^3$	$w_{Mn} = 2 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$
$\alpha \rightarrow \gamma$	$852.85°C \le \vartheta$ $\vartheta \le 877.85°C$	1126	$1.4 \cdot 10^{-8}$	$1.2 \cdot 10^3$	$w_{Mn} = 3 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$
$\gamma \rightarrow \alpha$	$852.85°C \le \vartheta$ $\vartheta \le 877.85°C$	1126	$1 \cdot 10^{-6}$	$-1.2 \cdot 10^3$	$w_{Mn} = 3 \cdot 10^{-3}$; $w_C = 2 \cdot 10^{-4}$

Effective mobility



Comparison with experimental data

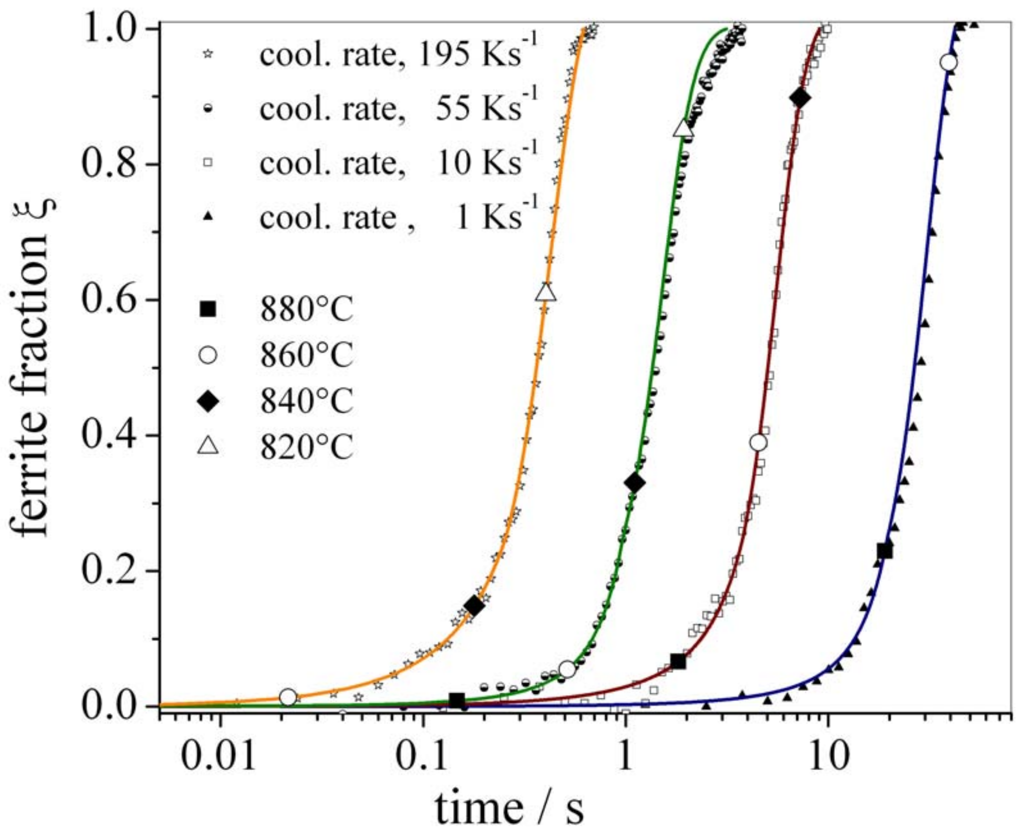


Table 1
Chemical composition of the investigated steel

C	Mn	P	S	Si	Ti	Nb	Al	N
0.002	0.11	0.01	0.008	0.01	0.059	0.009	0.033	0.0041

Values are mass fractions in %.

$$\xi(t) = \frac{a}{1 + b\exp(-ct)}$$

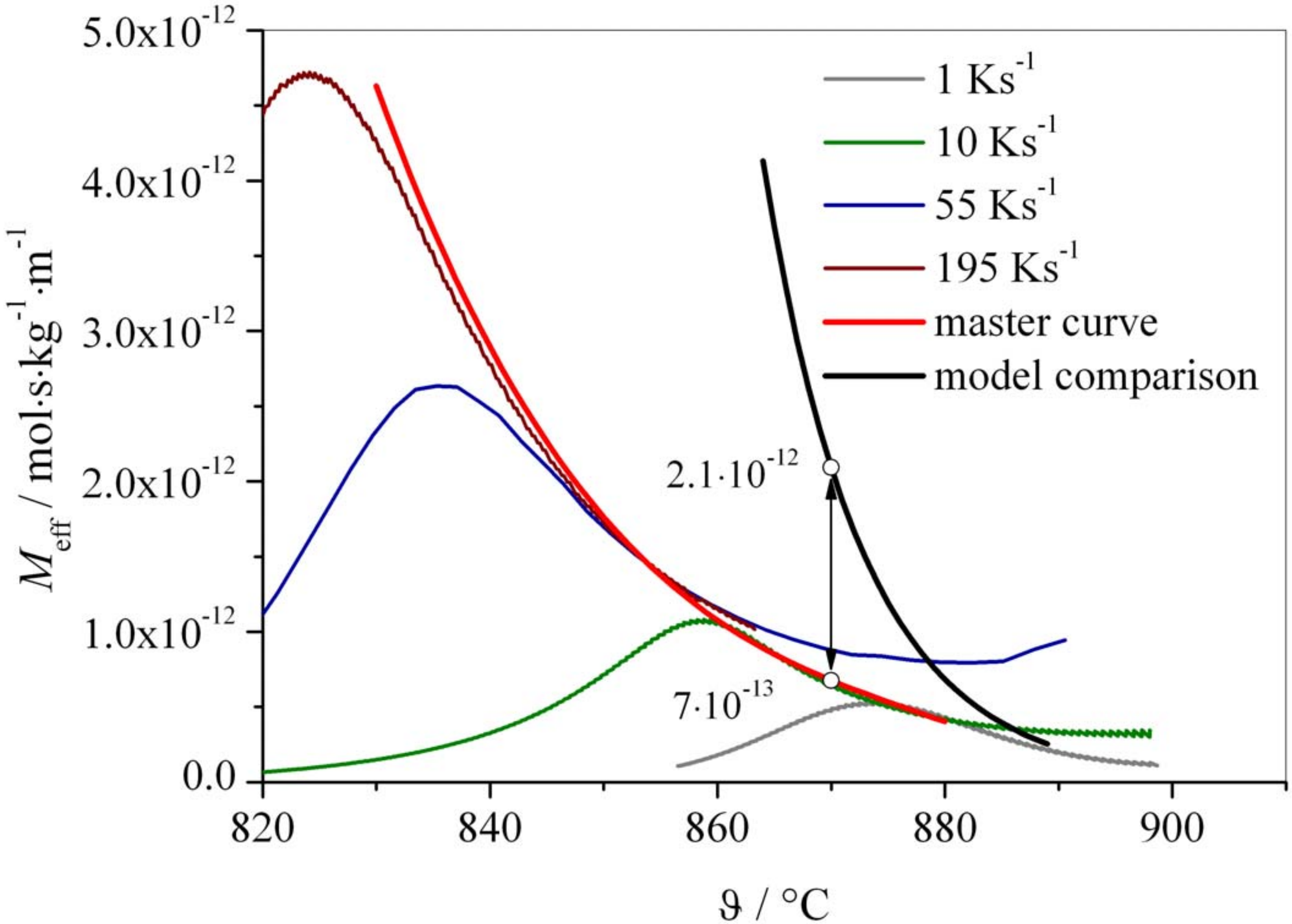
$$\frac{d\xi}{ds} \cdot \frac{ds}{dt} = \frac{d\xi}{ds}(\text{geometry}) \cdot \frac{ds}{dt}$$

$$v = M_{\text{eff}} \cdot \Delta G$$

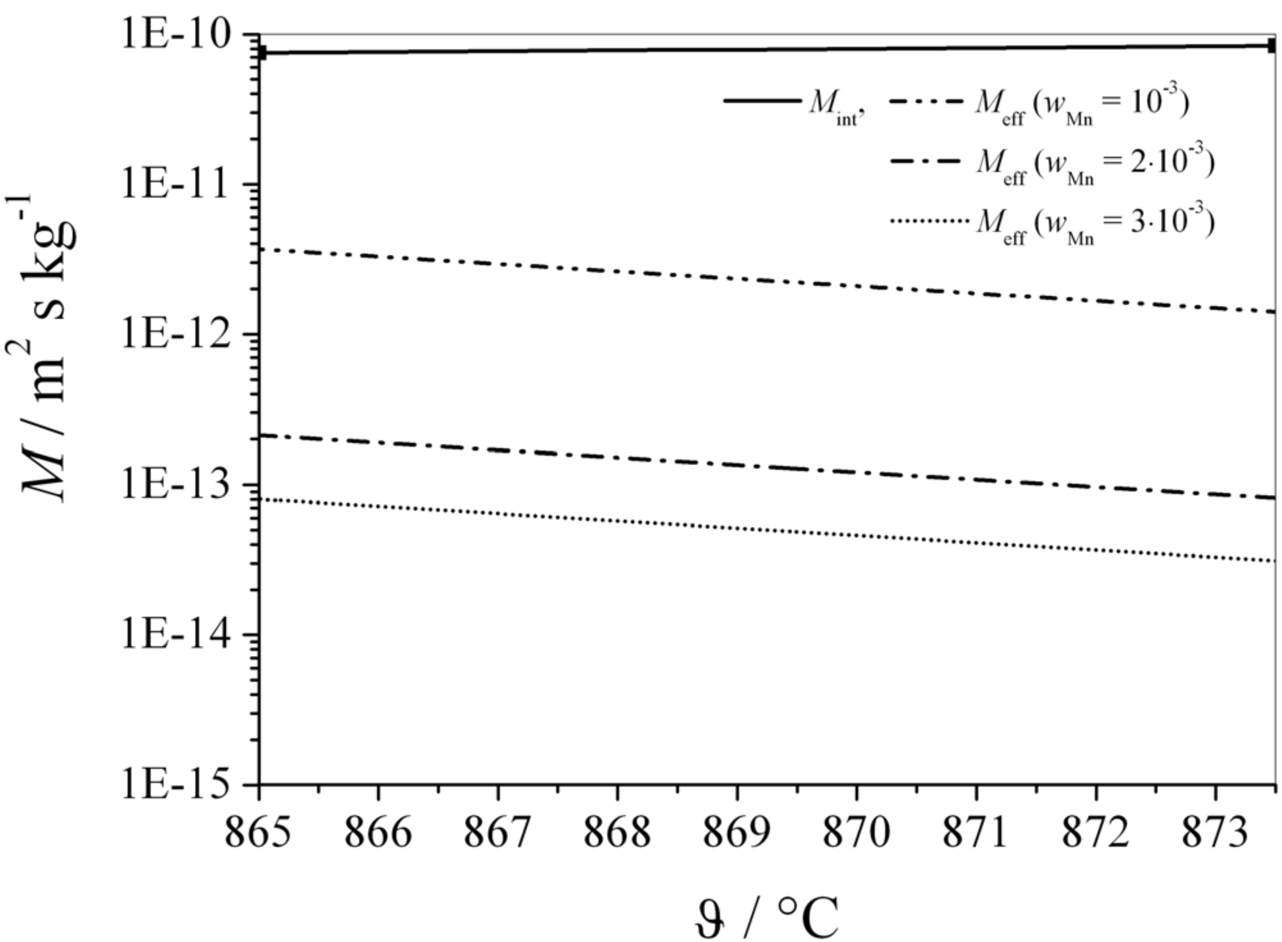
M. Militzer, Austenite decomposition kinetics in advanced low carbon steels, Solid Phase Transformations 99, eds. M. Koiwa, K. Otsuka and T. Miyazaki, JIM, Sendai (1999) 1521-1524.

E. Gamsjäger, M. Militzer, F. Fazeli, J. Svoboda, F. D. Fischer: "Interface mobility in case of the austenite-to-ferrite phase transformation", *Comp. Mat. Sci*, (2006) 94 -100.

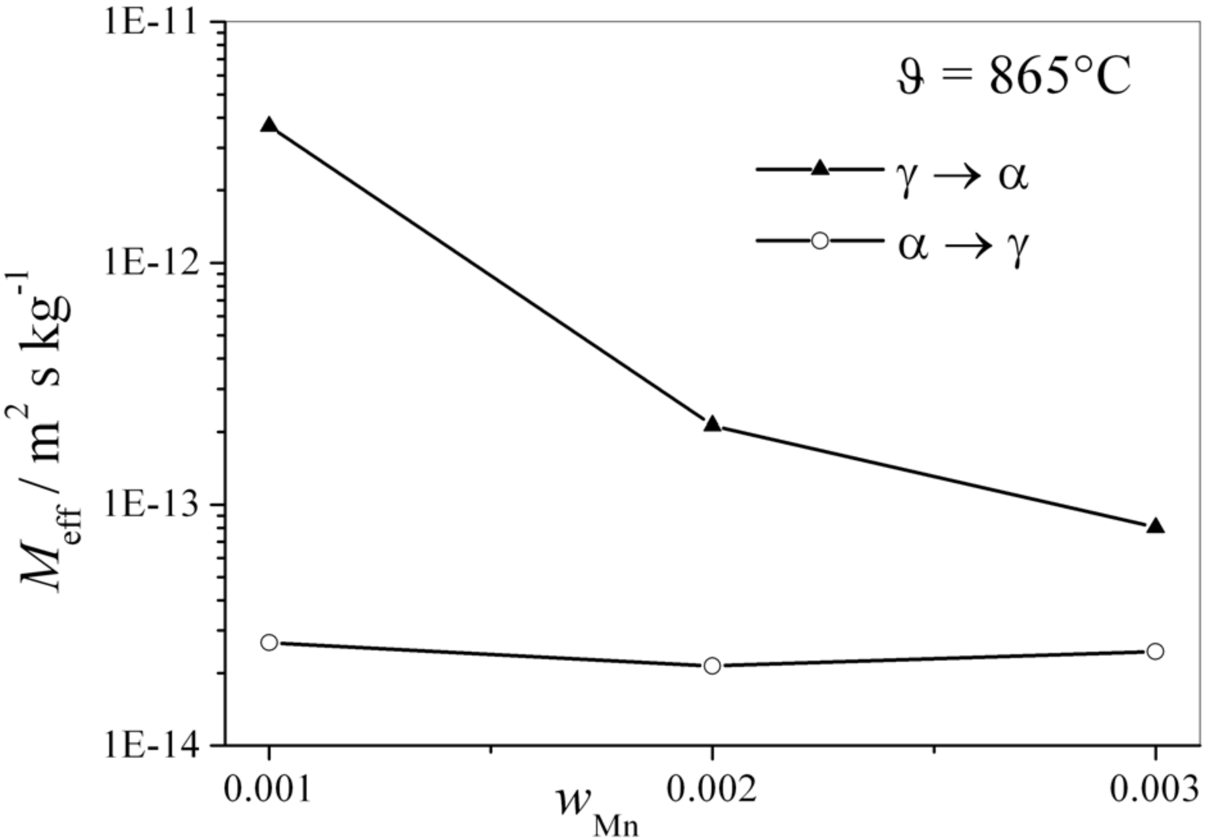
Comparison with experimental data



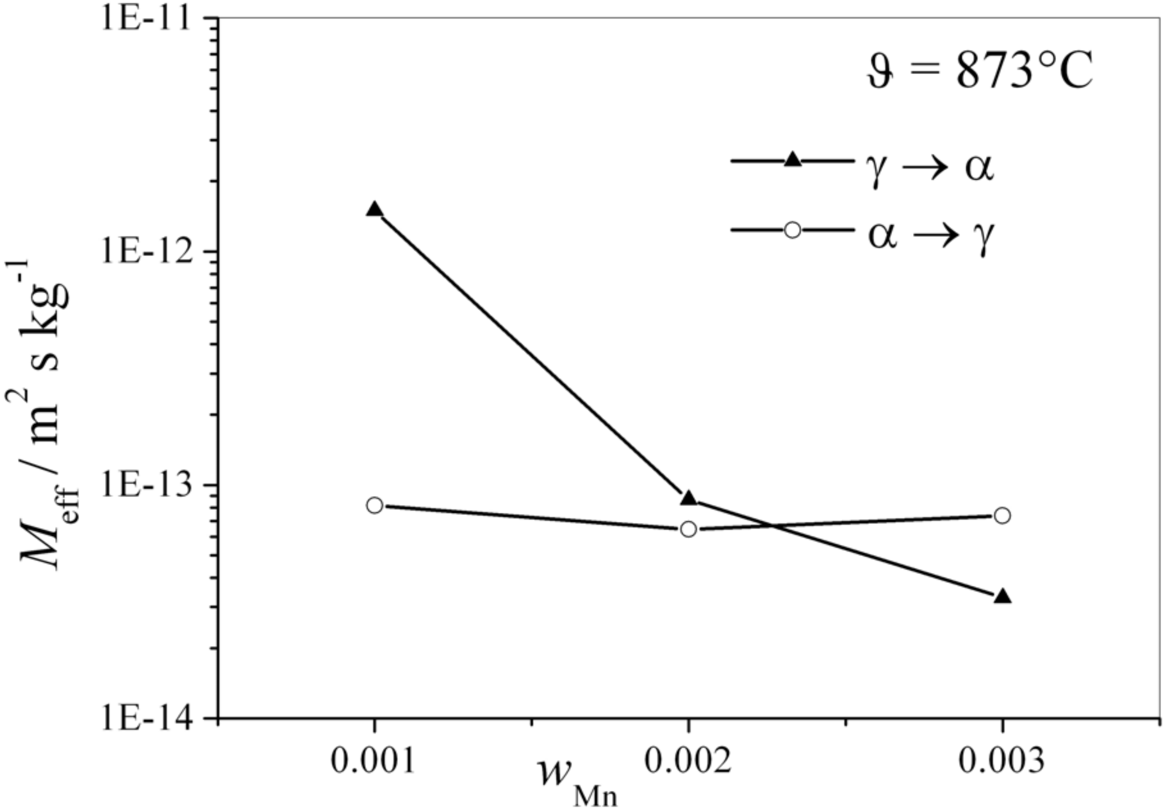
Comparison with intrinsic mobility



[1] M. Hillert, L. Höglund, Scrip. Mater. (2006), 54, 1259-1263.
[2] E. Gamsjäger, Habilitation treatise (2008), Montanuniversität Leoben



1E-11
1E-12
1E-13
1E-14
ϑ = 865°C
γ → α
α → γ
M_{eff} / m^2 s kg^{-1}
0.001
0.002
0.003
w_{Mn}



ϑ = 873°C
γ → α
α → γ
1E-11
1E-12
1E-13
1E-14
M_{eff} / m^2 s kg^{-1}
0.001
0.002
0.003
w_{Mn}

Conclusions and Outlook

- **Thick interface parametric model**
  - *Substitutional diffusion in the interface*
  - *C-diffusion in bulk*

  } *are rate-controlling.*

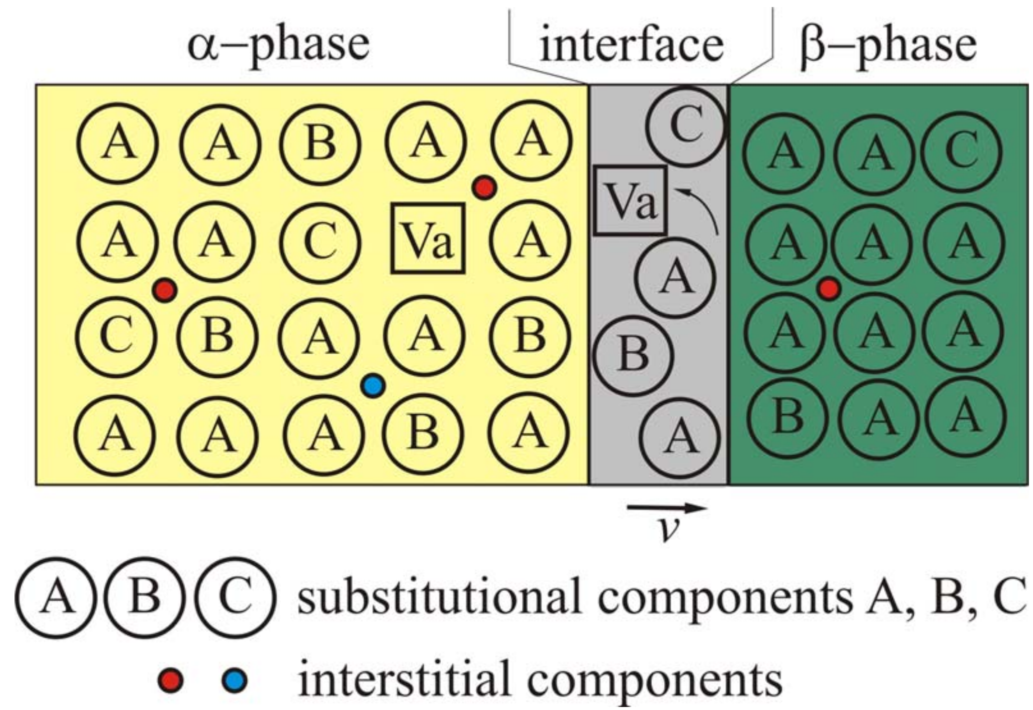
- **Simplified model**
  - *Comparison with experimental results.*

- **Prediction of the γ / α transformation kinetics**
  - *Effective mobility as a function of composition and temperature by comparison with LE-model and experiments.*

Kinetics of diffusive phase transformations

Transformation kinetics depends on:
1, Diffusion processes of the components in the bulk materials,
2, the rearrangement of the lattice and
3, on diffusion processes in the interface.

2+3: interfacial reaction



Gibbs energy *G* and dissipation *Q*

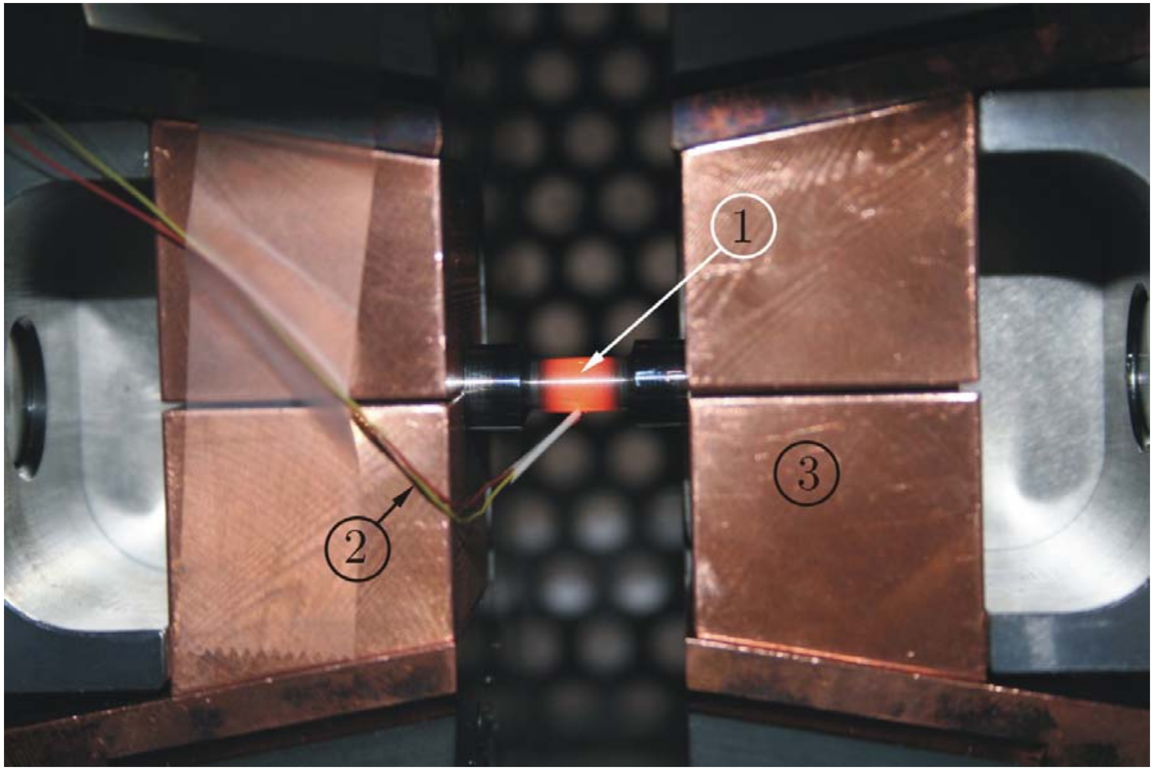
$$G = \frac{1}{\Omega}\int_{-\Delta_L - h}^{\Delta_R}\left(x\mu_1 + (1-x)\mu_2\right)\mathrm{d}z = \underbrace{\frac{1}{\Omega}\int_{-\Delta_L - h}^{0}\left(x\mu_1 + (1-x)\mu_2\right)\mathrm{d}z}_{G^{\alpha+I}} + \underbrace{\frac{1}{\Omega}\int_{0}^{\Delta_R}\left(x\mu_1 + (1-x)\mu_2\right)\mathrm{d}z}_{G^{\beta}}$$

$$Q = RT\Omega \int_{-(\Delta_L + h)}^{\Delta_R}\left(\frac{1}{xD_1} + \frac{1}{(1-x)D_2}\right) j^2 dz$$

$$G = G(x_L,\ x_R,\ A,\ \Delta_R) \qquad Q = Q(\dot{x}_L,\ \dot{x}_R,\ \dot{A},\ v)$$

$$\frac{1}{2}\frac{\partial Q}{\partial \dot{x}_L} = -\frac{\partial G}{\partial x_L} \qquad \frac{1}{2}\frac{\partial Q}{\partial \dot{x}_R} = -\frac{\partial G}{\partial x_R} \qquad \frac{1}{2}\frac{\partial Q}{\partial v} = \frac{\partial G}{\partial \Delta_R} \qquad \frac{1}{2}\frac{\partial Q}{\partial \dot{A}} = -\frac{\partial G}{\partial A}$$

Experimental setup



1... Heated specimen
2 ... Electric supply for the thermocouple
3 ... Cu jaws

Composition, heat treatment and microstructure

Table: Composition of the 10MnSi7 steel grade

	C	Mn	Si	P	S	Cr	Ni	Al	Ti	V	Nb
$x_i \cdot 100$	0.4173	1.6259	1.9802	0.0219	0.0124	0.0318	0.0188	0.0592	0.0460	0.0054	0.0018