Phase field modeling of ferrite growth in Fe-C-Mn steels

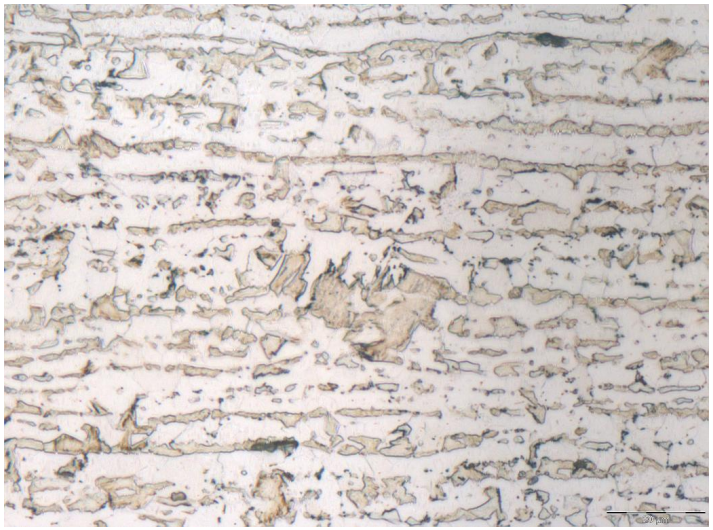
Alexandre Viardin [1]
Benoît Appolaire [2]
Elisabeth Aeby-Gautier [1]
Mohamed Gouné [3]

[1] École des Mines de Nancy, France
[2] LEM, Onera-CNRS, France
[3] Arcelor Mittal Research

Motivation

Martensite banding in dual phase steels

[Grange, Metallurgical Transactions 2 (1971) 417]



[B. Krebs, A. Hazotte, M. Gouné]

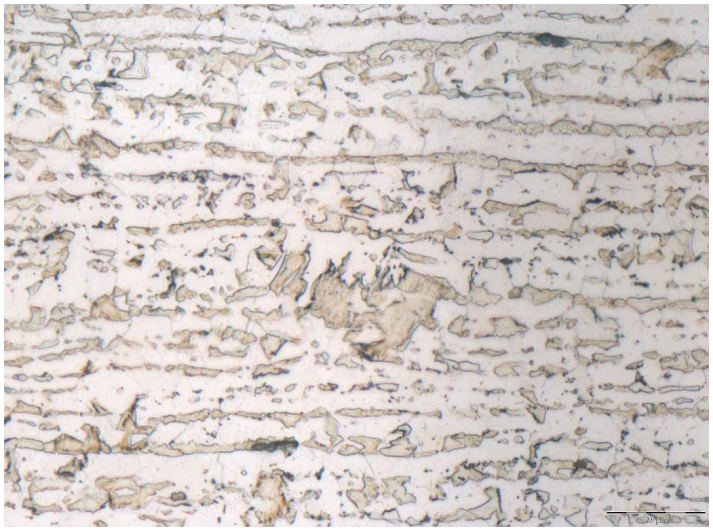
- Mn Microsegregation
- After thermomechanical process of dual phase steels, martensite banding is likely to appear
- This morphology is detrimental to mechanical properties

- Role of ferrite *growth* on the banding or is *nucleation* sufficient to explain everything ?

Motivation

Martensite banding in dual phase steels

[Grange, Metallurgical Transactions 2 (1971) 417]



[B. Krebs, A. Hazotte, M. Gouné]

- Mn Microsegregation
- After thermomechanical process of dual phase steels, martensite banding is likely to appear
- This morphology is detrimental to mechanical properties

- Phase field could be well suited for that purpose . . .
- . . . provided that kinetics is properly predicted

Motivation

Different Growth Modes ($D_{\mathrm{Mn}} \ll D_{\mathrm{C}}$)

[Coates, Metallurgical Transactions 3 (1972) 1203]

1. Orthoequilibrium
   - Local Equilibrium with Partitioning (LEP)
   - Local Equilibrium with Non Partitioning (LENP)
2. Paraequilibrium
3. Transitions between the different regimes

Is that straightforward to account for with phase field ?

Phase field Model

Mixing *Kim, Kim, Suzuki* and *Warren, Kobayashi, Craig Carter*

[Kim et al., Phys. Rev. E 60 (1999) 7186], [Warren et al., Acta Mater. 51 (2003) 6035]

$$\mathcal{F} = \int_\Omega \left(f_0(\phi, c_i^\alpha, c_i^\gamma) + \frac{\epsilon^2}{2} |\nabla \phi|^2 + \chi \left[1 - h(\phi) \right] |\nabla \psi| \right) \mathrm{d}\Omega$$

- Homogeneous free energy

$$f_0(\phi, c_i^\alpha, c_i^\gamma) = h(\phi) f^\gamma(c_i^\gamma) + [1 - h(\phi)] f^\alpha(c_i^\alpha) + W\, g(\phi)$$

- Arbitrary $f^\gamma(c_i^\gamma)$ and $f^\alpha(c_i^\alpha)$ (e.g. Calphad)
- No extra contribution of the concentration profile within the interface to the interfacial energy thanks to auxilliary c_i^ϕ
- Thin interface asymptotics analysis for determining M_ϕ

Phase field Model

Governing equations

$$\mathcal{F} = \int_\Omega \left(f_0(\phi, c_i^\alpha, c_i^\gamma) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) \, \mathrm{d}\Omega$$

$$\partial_t \phi = -M_\phi \left(\frac{\delta \mathcal{F}}{\delta \phi} \right)$$

$$\partial_t c_i = \nabla \cdot \left(L_{ij} \nabla \frac{\delta \mathcal{F}}{\delta c_j} \right)$$

Phase field Model

Governing equations

$$\mathcal{F} = \int_\Omega \left(f_0(\phi, c_i^\alpha, c_i^\gamma) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) \, \mathrm{d}\Omega$$

$$\partial_t \phi = -M_\phi \left(\epsilon^2 \, \Delta \phi - h' \, \Delta F_c - W \, g' \right)$$

$$\partial_t c_i = \nabla \cdot \left(L_{ij} \nabla \frac{\delta \mathcal{F}}{\delta c_j} \right)$$

Phase field Model

Governing equations

$$\mathcal{F} = \int_\Omega \left(f_0(\phi, c_i^\alpha, c_i^\gamma) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) \, \mathrm{d}\Omega$$

$$\partial_t \phi = -M_\phi \left(\epsilon^2 \, \Delta \phi - h' \, \Delta F_c - W \, g' \right)$$

$$\partial_t c_i = \nabla \cdot \left(L_{ij} \, \nabla \frac{\partial f_0}{\partial c_j} \right)$$

Phase field Model

Governing equations

$$\mathcal{F} = \int_\Omega \left(f_0(\phi, c_i^\alpha, c_i^\gamma) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) \, \mathrm{d}\Omega$$

$$\partial_t \phi = -M_\phi \left(\epsilon^2 \, \Delta \phi - h' \, \Delta F_c - W \, g' \right)$$

$$\partial_t c_i = \nabla \cdot \left(L_{ij} \, \nabla \frac{\partial f_0}{\partial c_j} \right)$$

supplied with:

$$c_i = h(\phi) \, c_i^\alpha + [1 - h(\phi)] \, c_i^\gamma$$

$$\frac{\partial f^\alpha}{\partial c_i^\alpha} = \frac{\partial f^\gamma}{\partial c_i^\gamma}$$

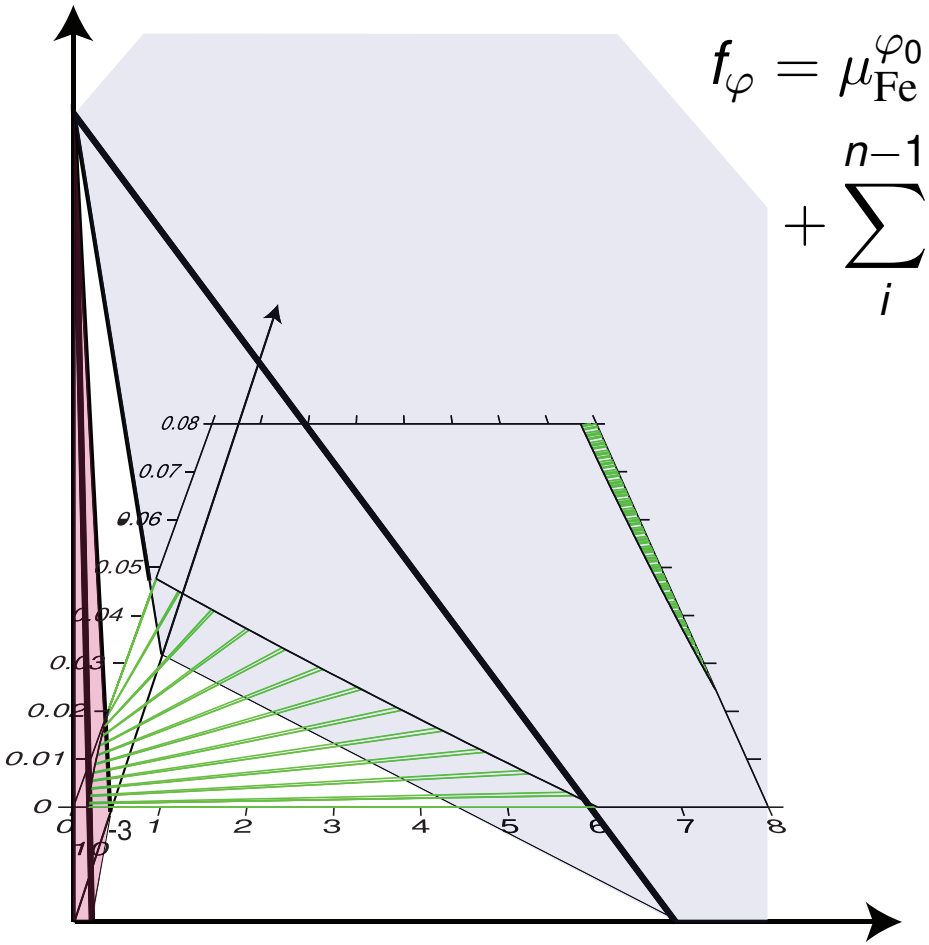
similar to homogenization schemes

[Ammar et al., Eur. J. Comp. Mech. (2010)]

Talk K. Ammar (thursday, Benoît XII)

Phase field Model

Linearized phase diagram



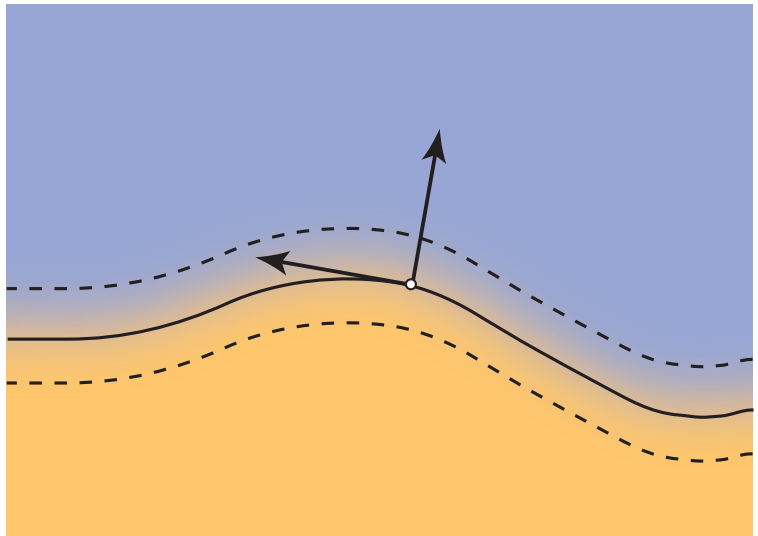
$$f_\varphi = \mu_{\mathrm{Fe}}^{\varphi 0}(T,p) - p\,v_{\mathrm{m}} + \sum_i^{n-1} c_i^\varphi \left[\mu_i^{\varphi 0}(T_a,p)\,RT_a\left(a_i \ln c_i^\varphi - 1\right) + \epsilon_{\mathrm{Fei}}^\varphi \right]$$

- free parameters $\mu_{\mathrm{Fe}}^{\varphi 0}$, $\delta\mu_i + \delta\epsilon_{\mathrm{Fei}}$ and a_i
- to set m_{C}, m_{Mn}, k_{C}, k_{Mn}

Phase field Model

Asymptotics analysis (over-simplified) Poster Y. Le Bouar

- local frame
- expansions of the fields (ϕ,c_i^ϕ ...)



- Order 0 (conventional analysis)

$$\phi(x) = \tfrac{1}{2}\left(1 - \tanh \xi\right)$$
$$c^{\alpha(0)} = c_{\mathrm{eq}}^{\alpha}$$
$$c^{\gamma(0)} = c_{\mathrm{eq}}^{\gamma}$$

- Order 1

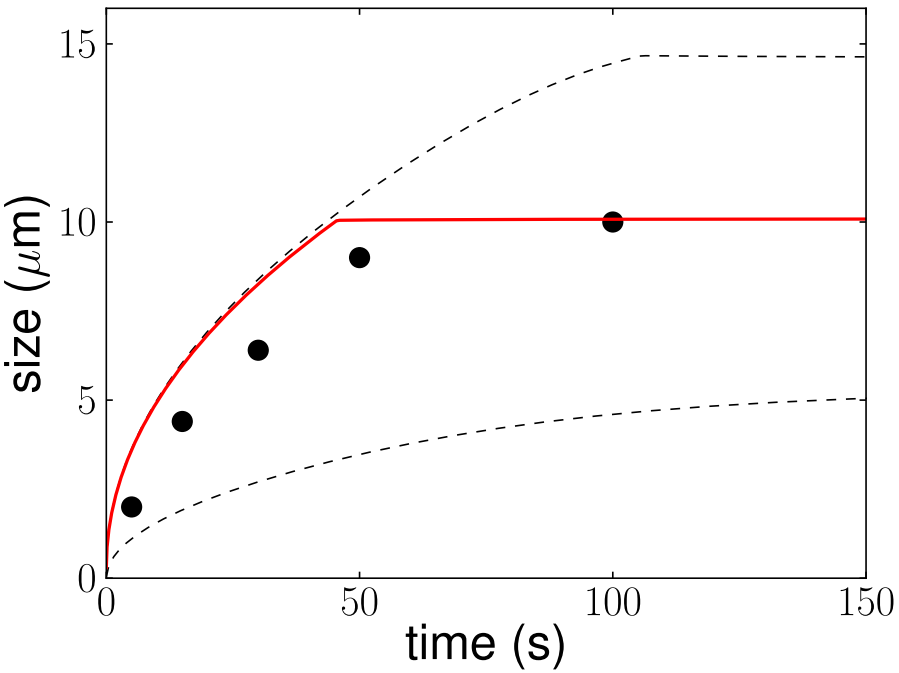
$$\frac{1}{M_\phi} = \frac{\epsilon^3}{\sigma\sqrt{2W}}\left\{\frac{1}{D_{\mathrm{C}}^{\gamma}}\zeta_C + \frac{1}{D_{\mathrm{Mn}}^{\gamma}}\zeta_{Mn}\right\}$$

Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



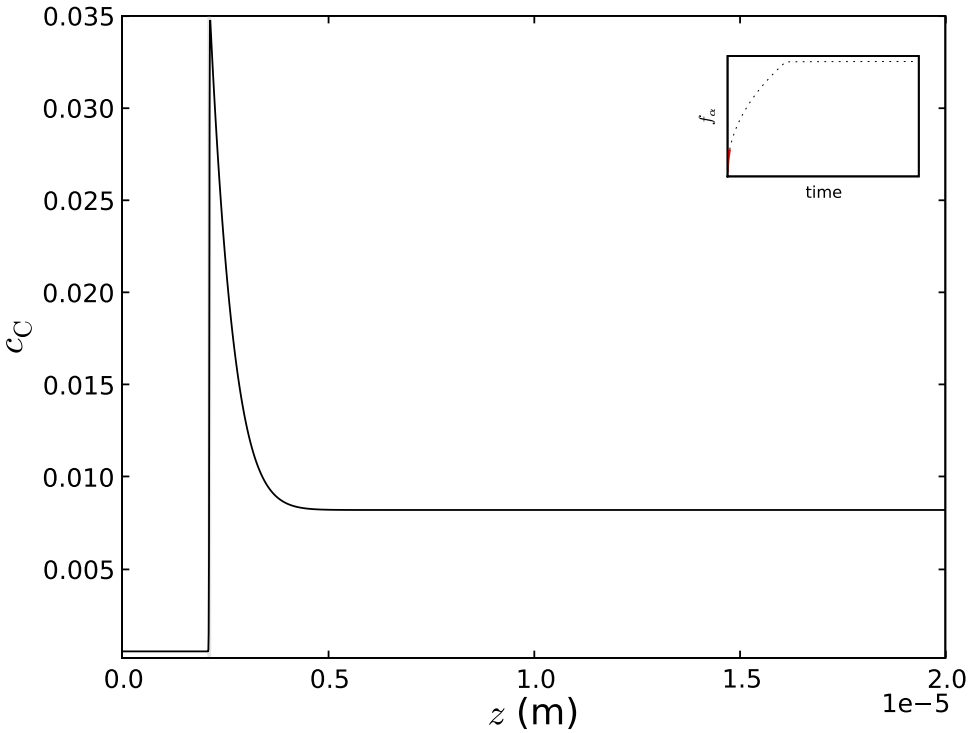
- Measured kinetics is faster than orthoequilibrium (NPLE)
- Measured kinetics stops below paraequilibrium fraction
- Good agreement between phase field and experiments

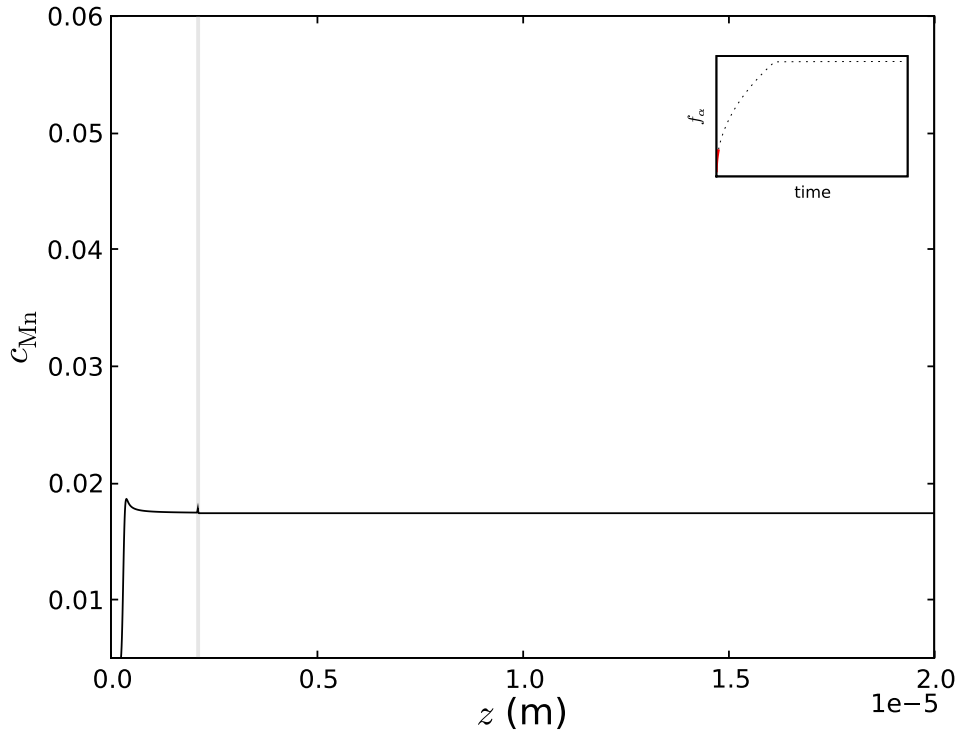
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



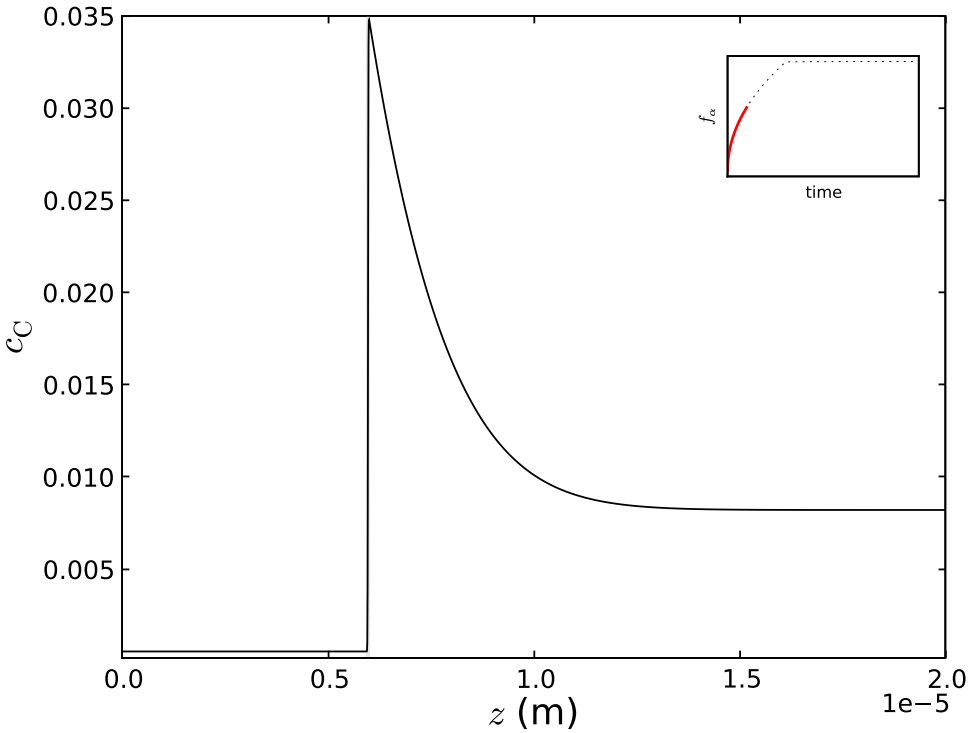


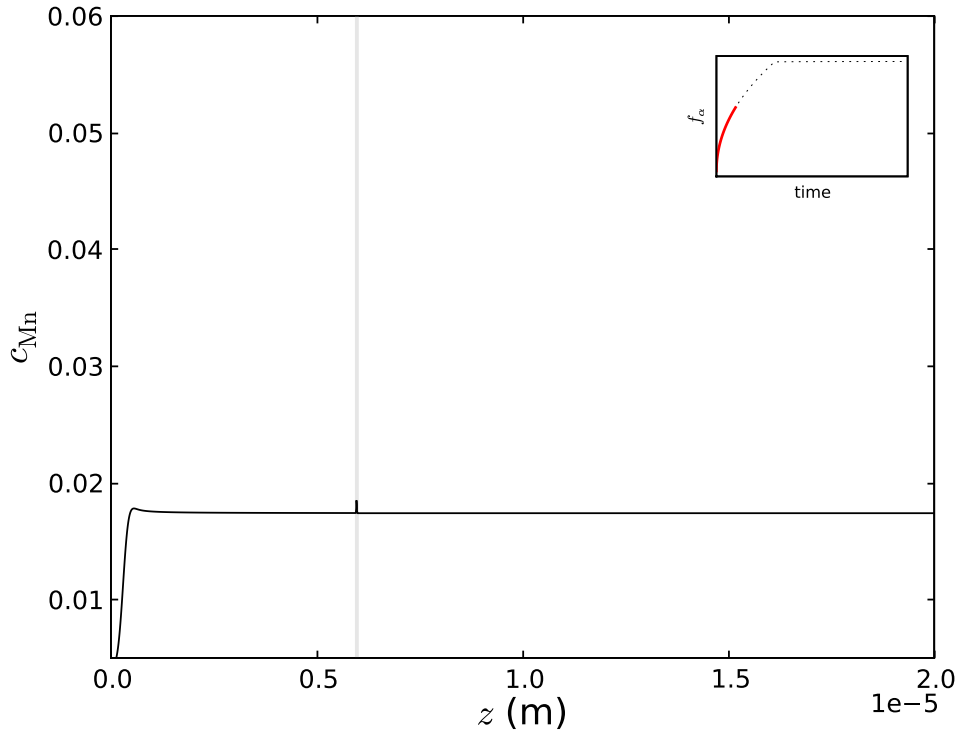
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



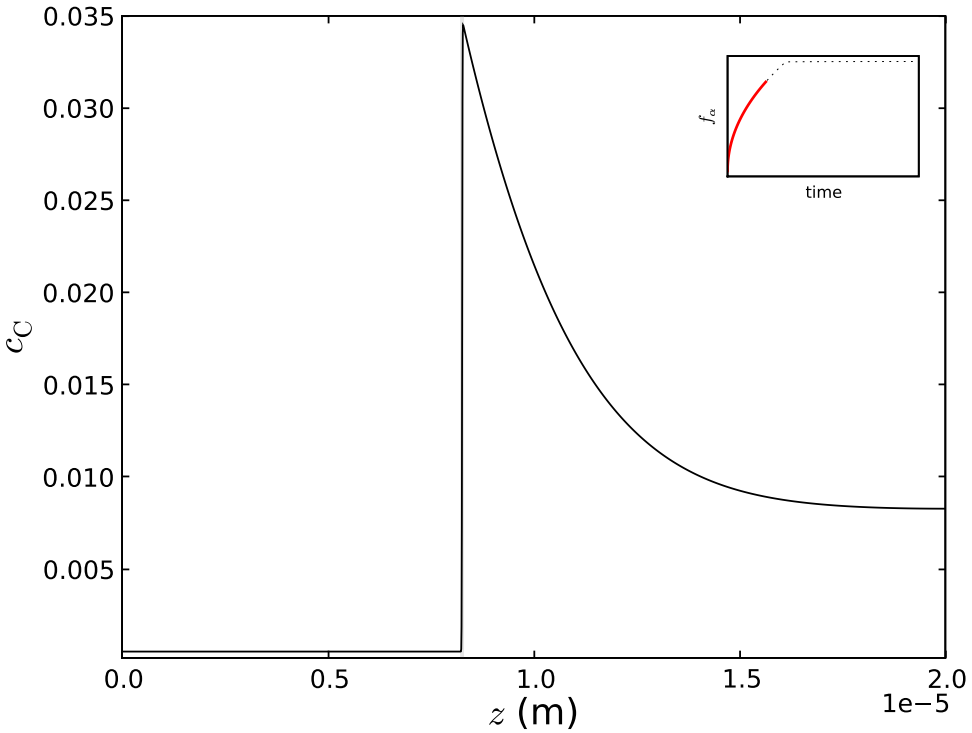


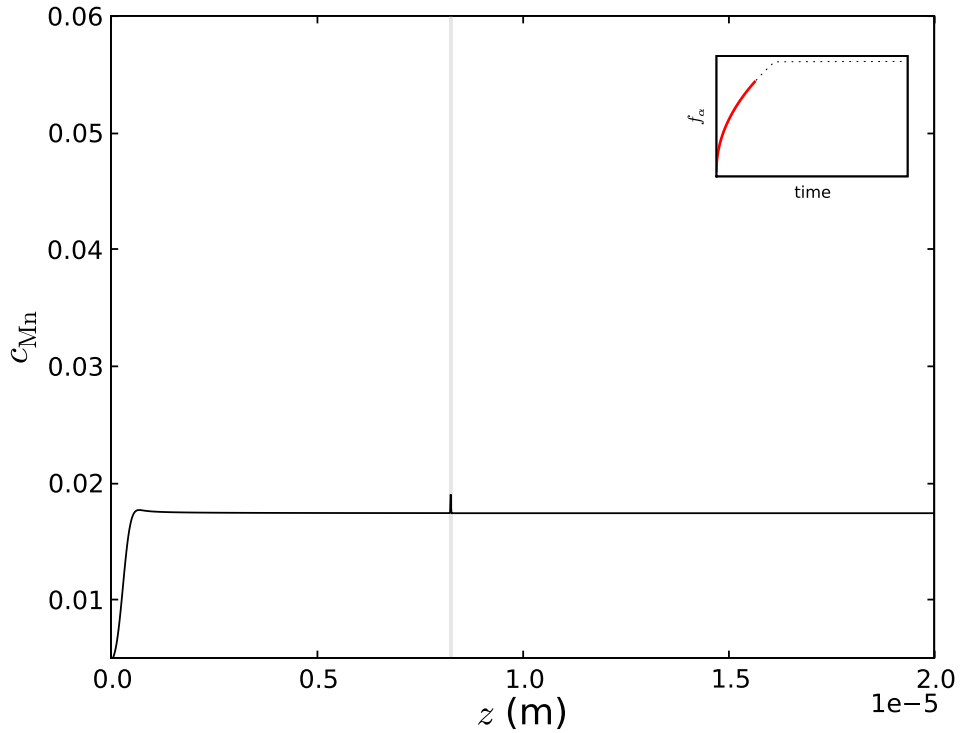
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



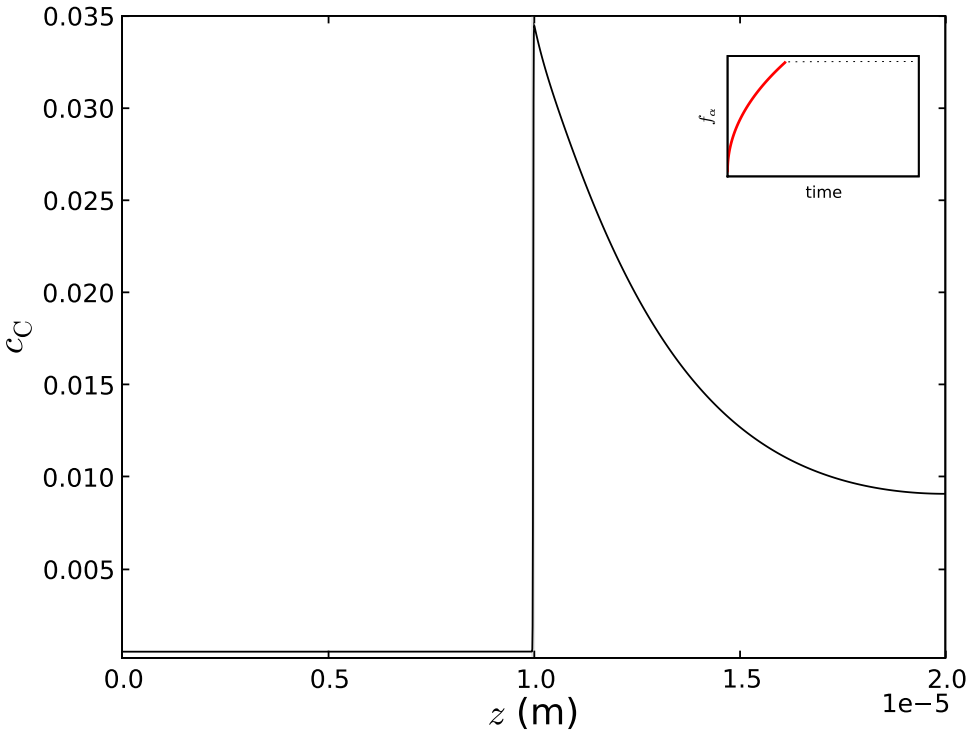


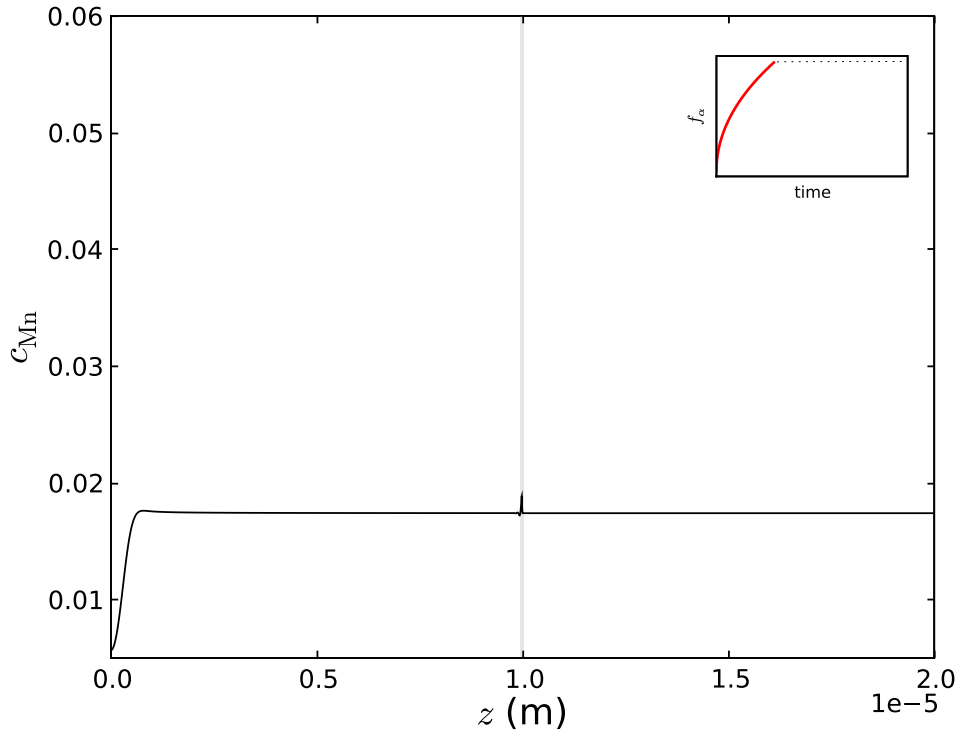
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



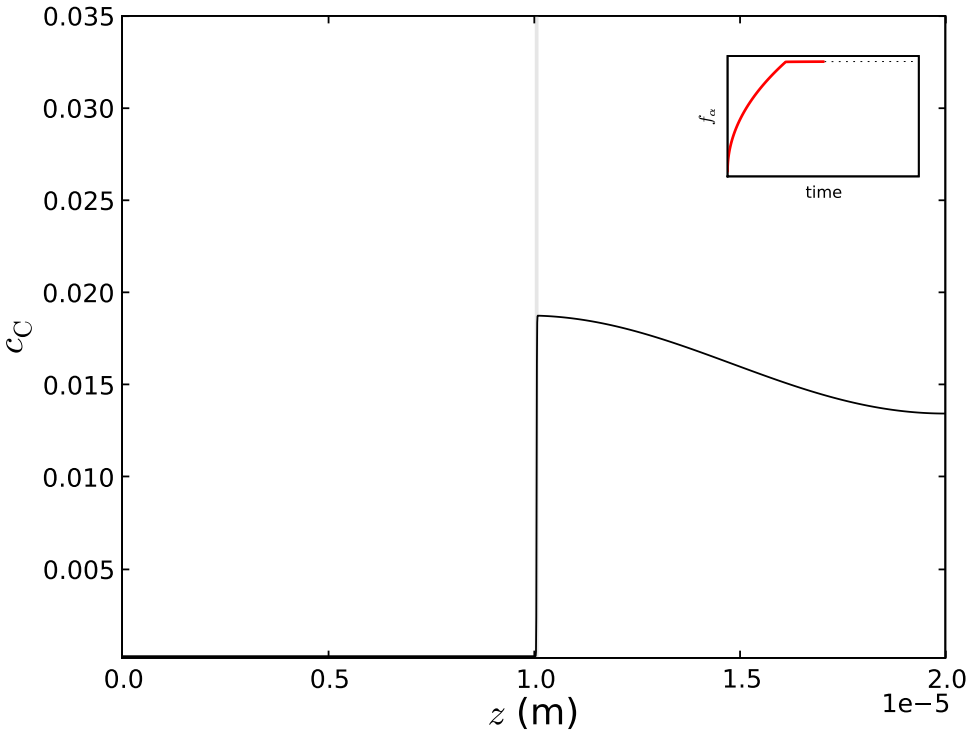


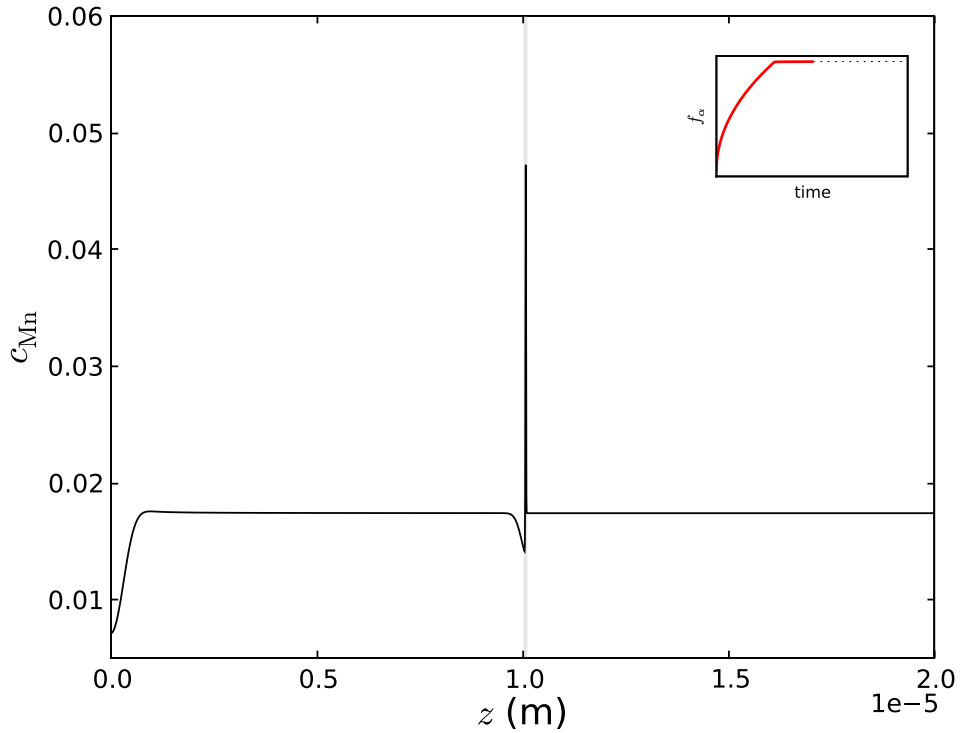
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



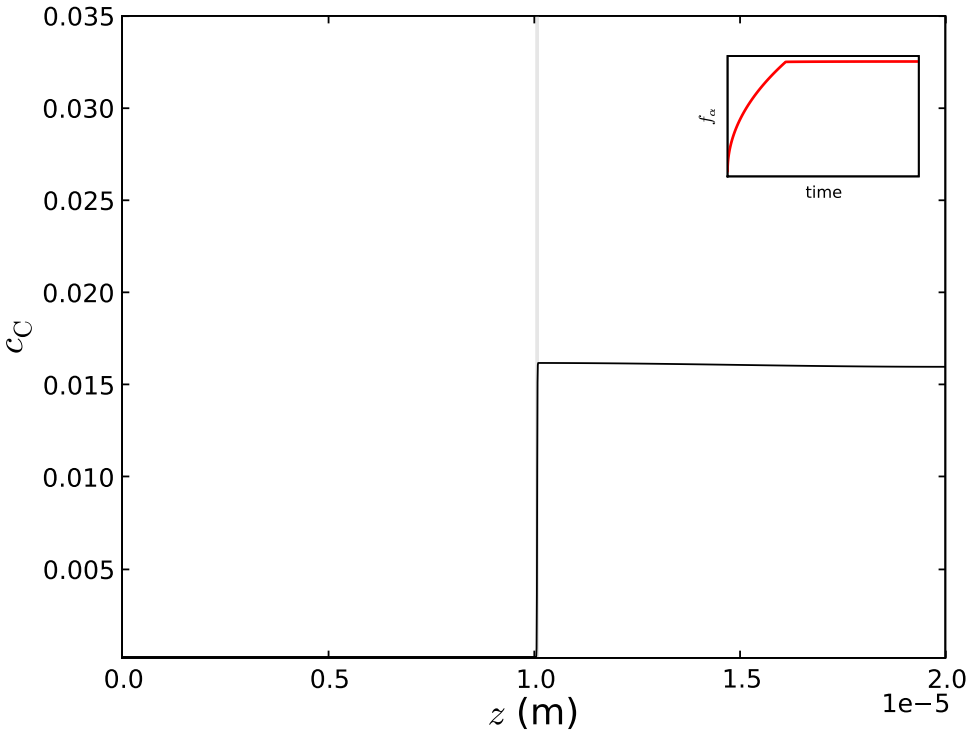


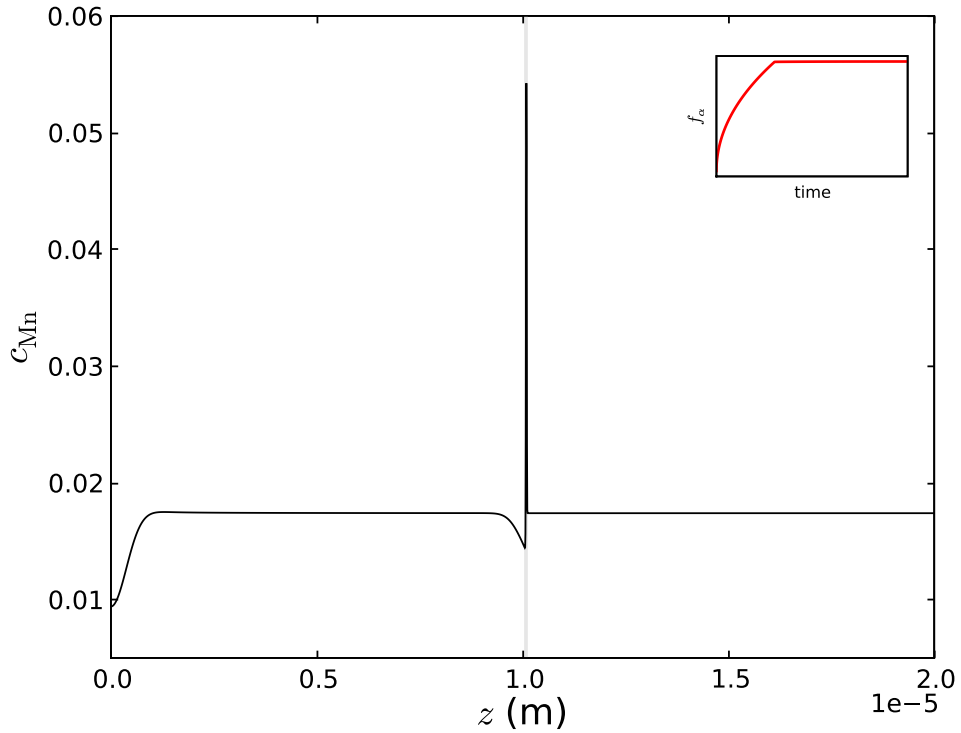
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



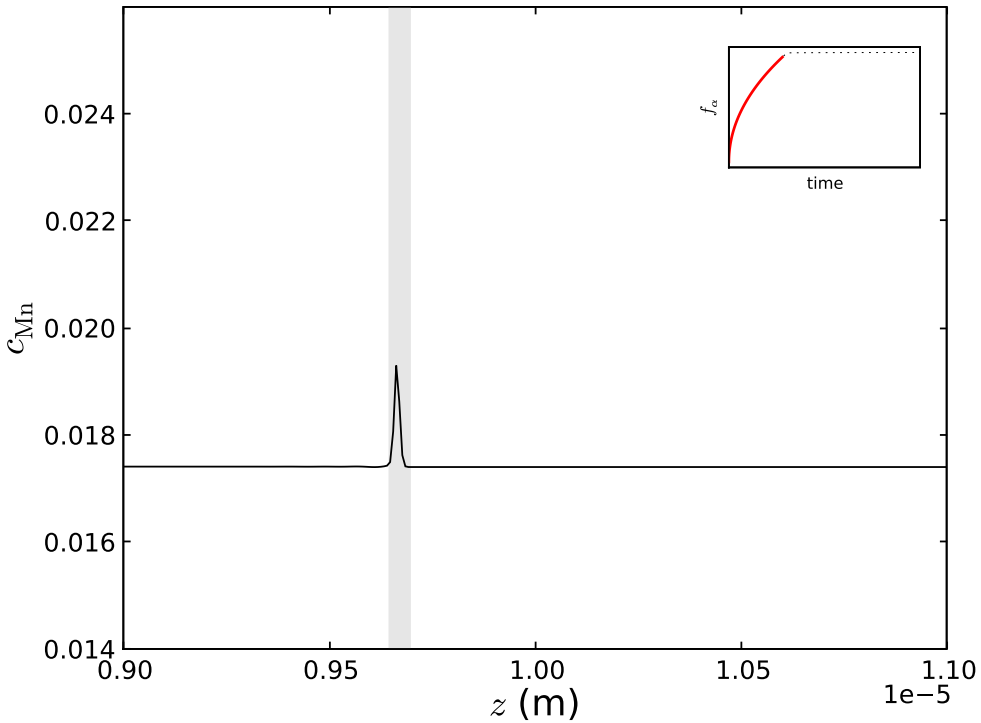


Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C

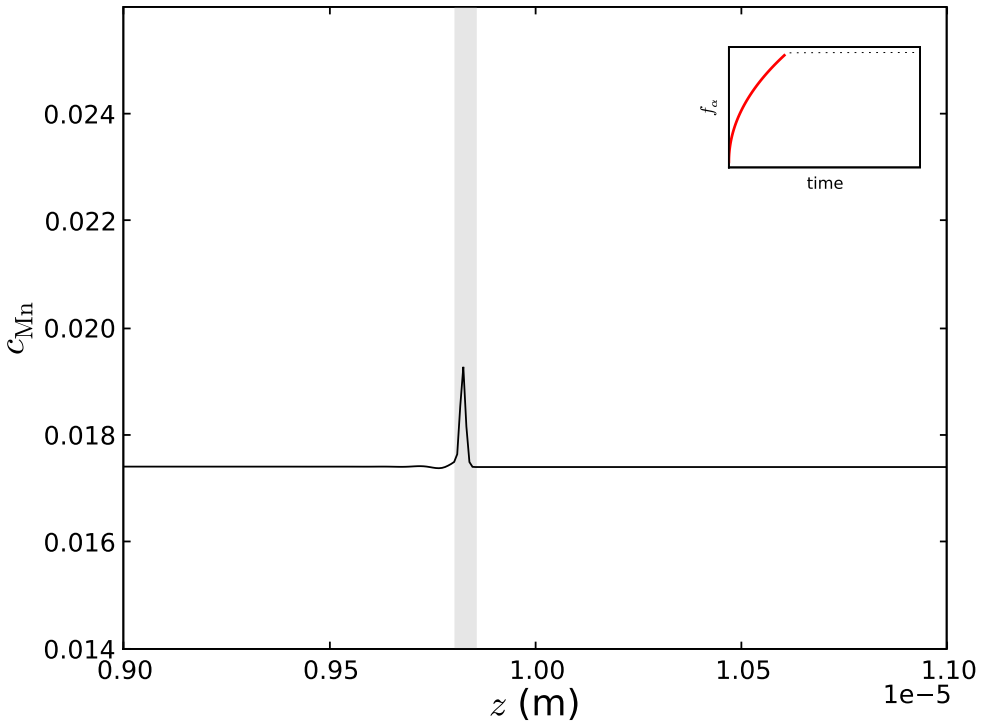


Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C

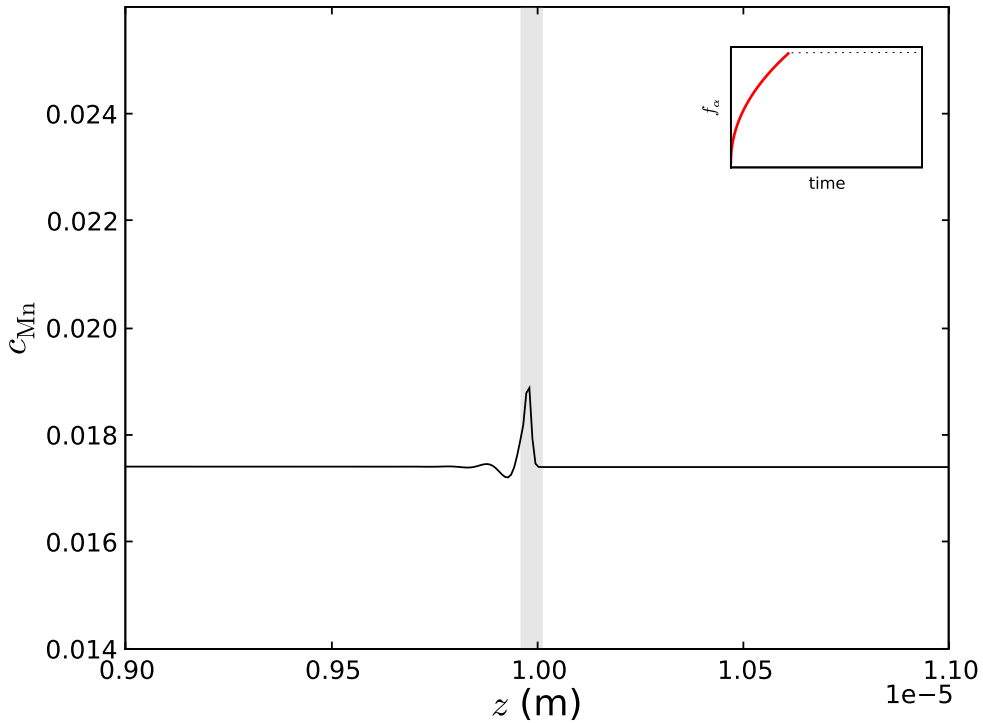


Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C

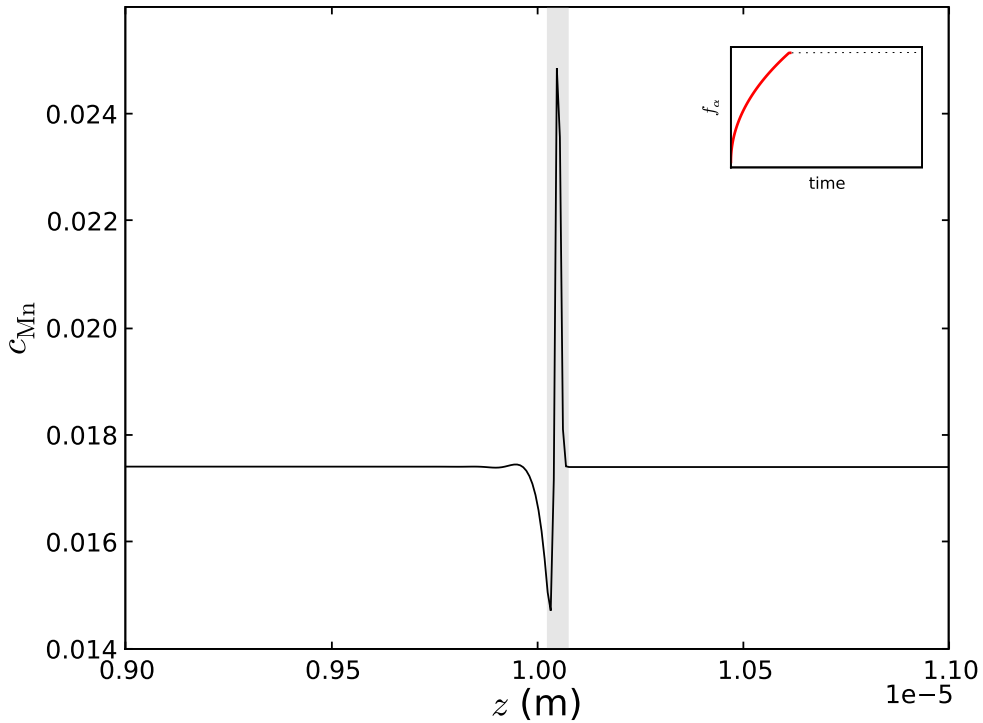


Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C

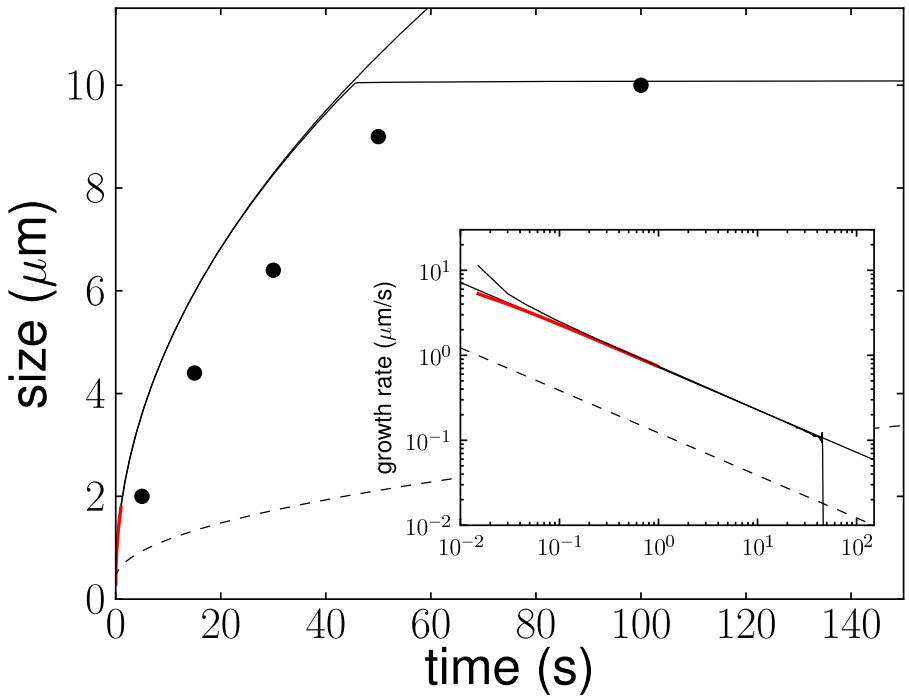


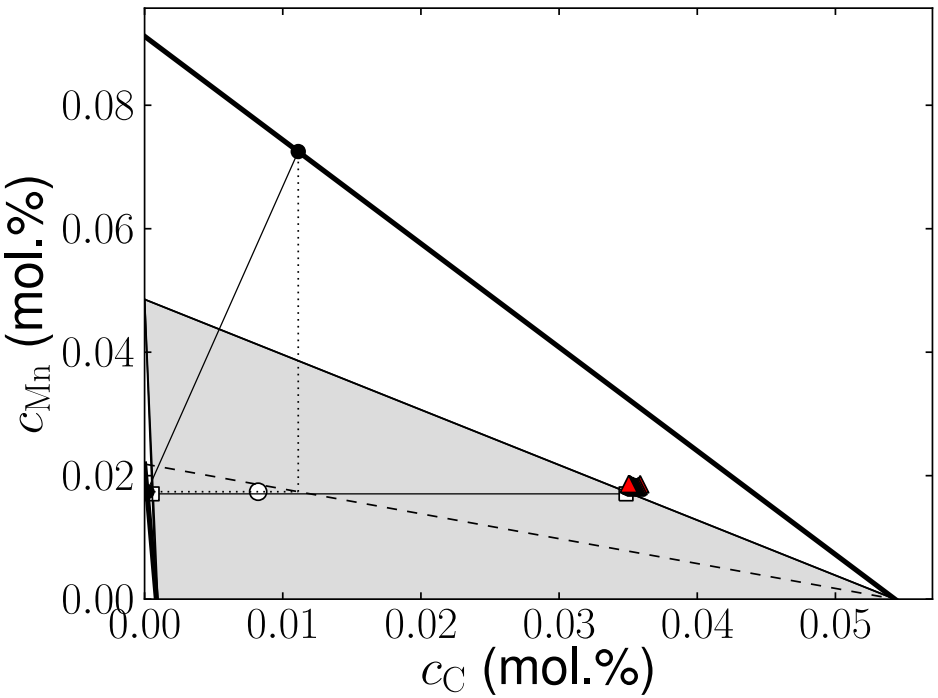
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



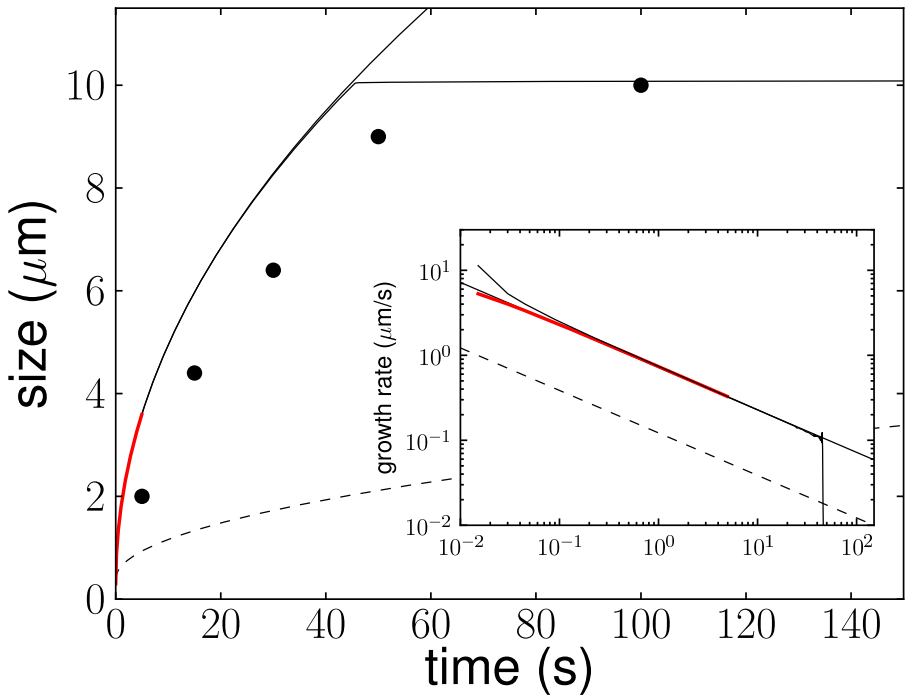


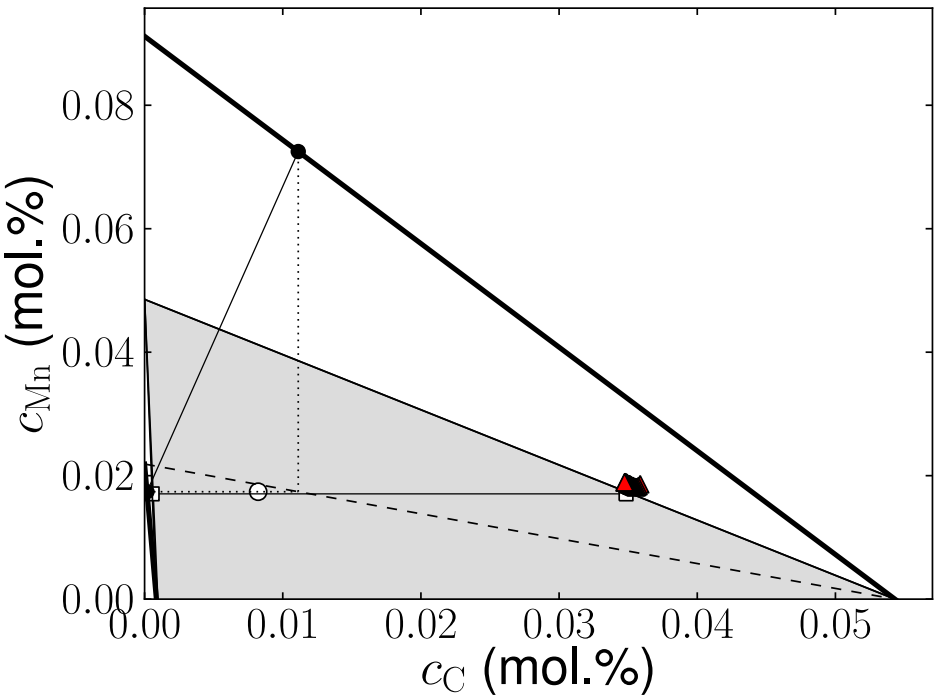
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



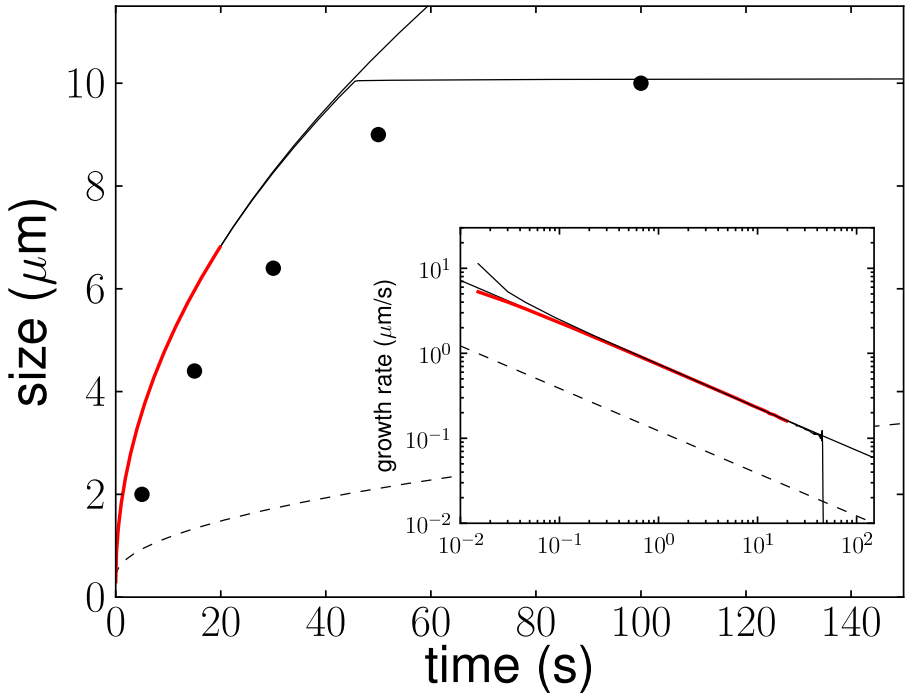


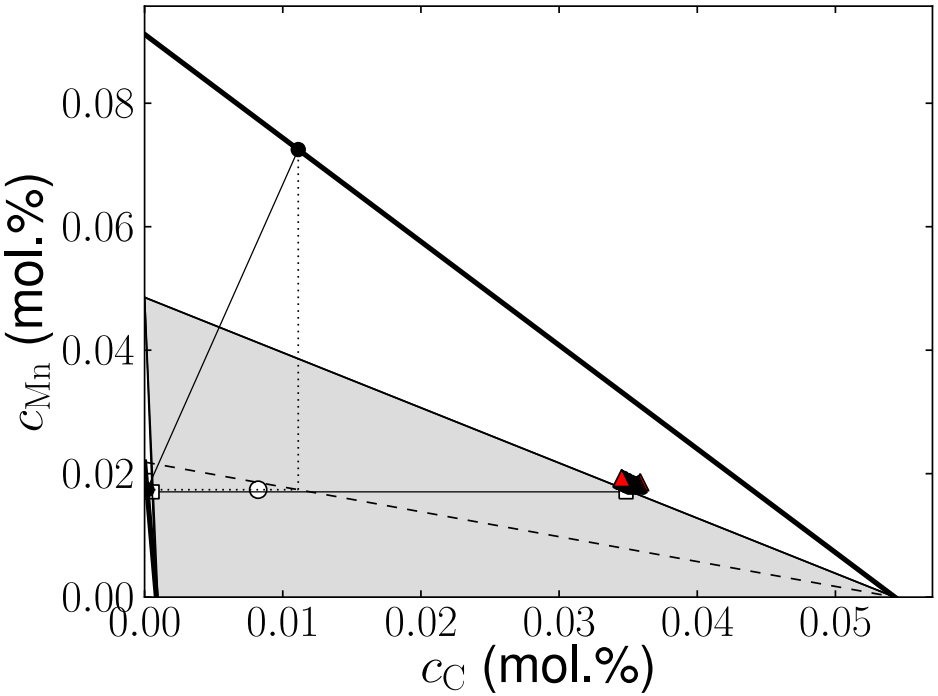
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



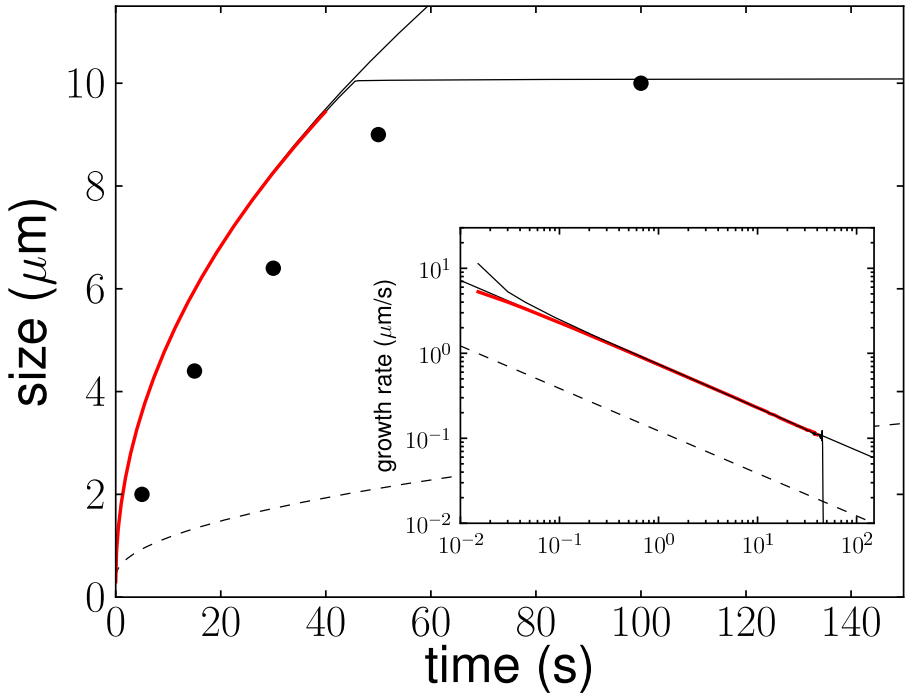


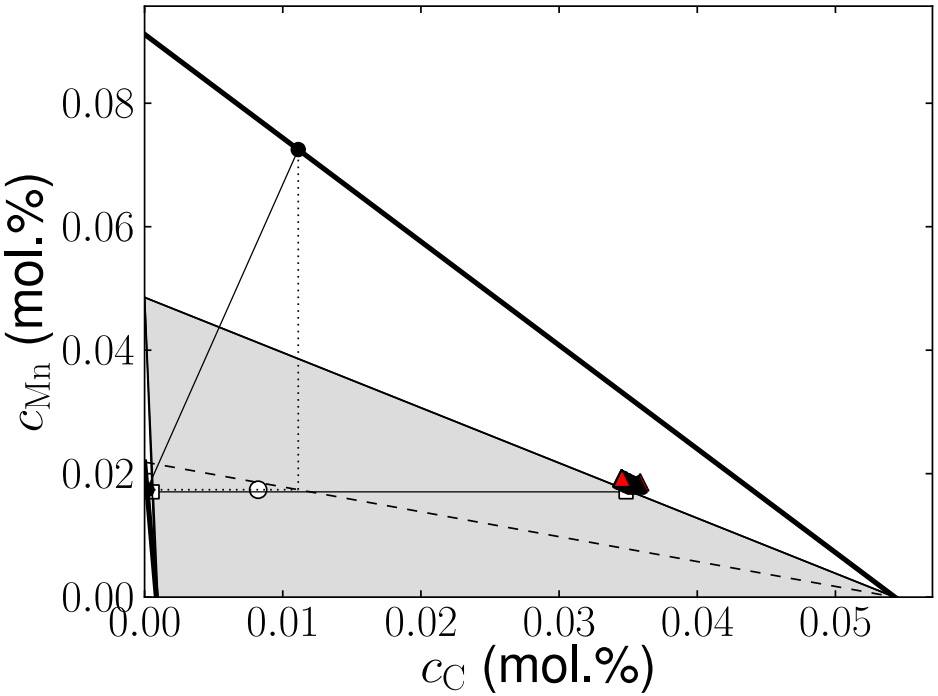
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



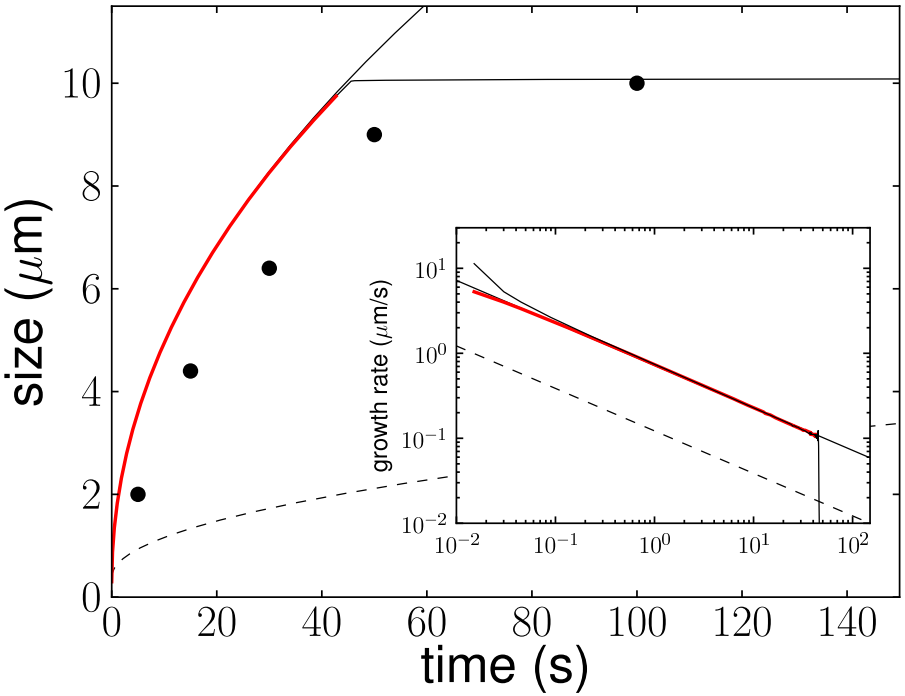


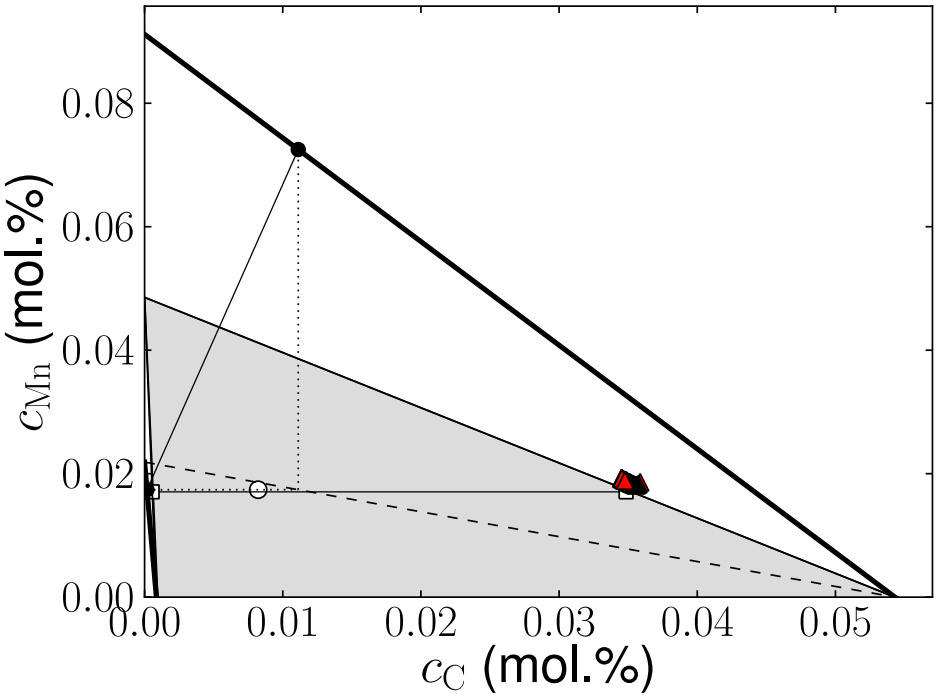
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



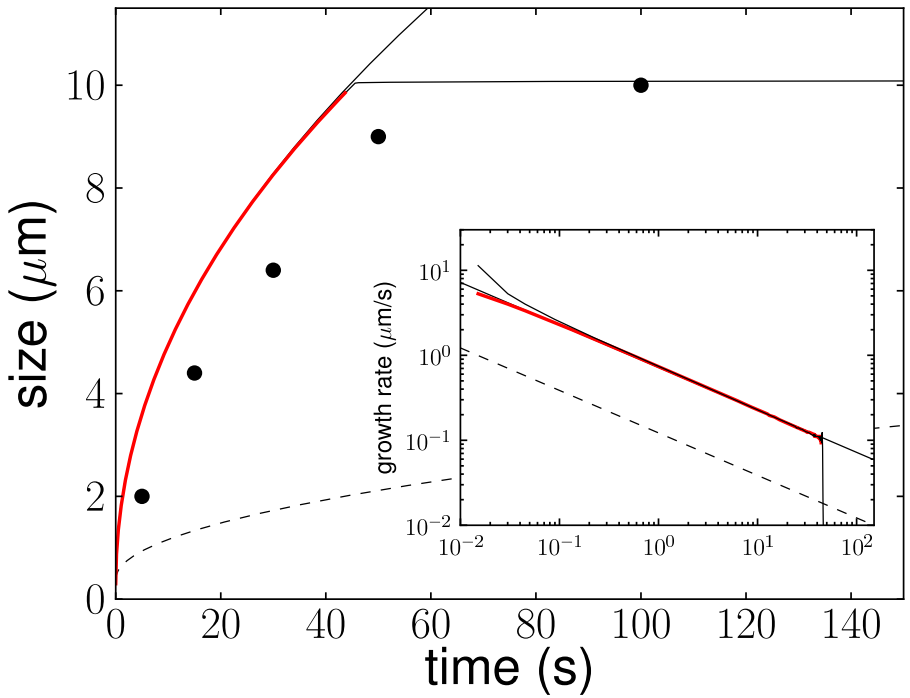


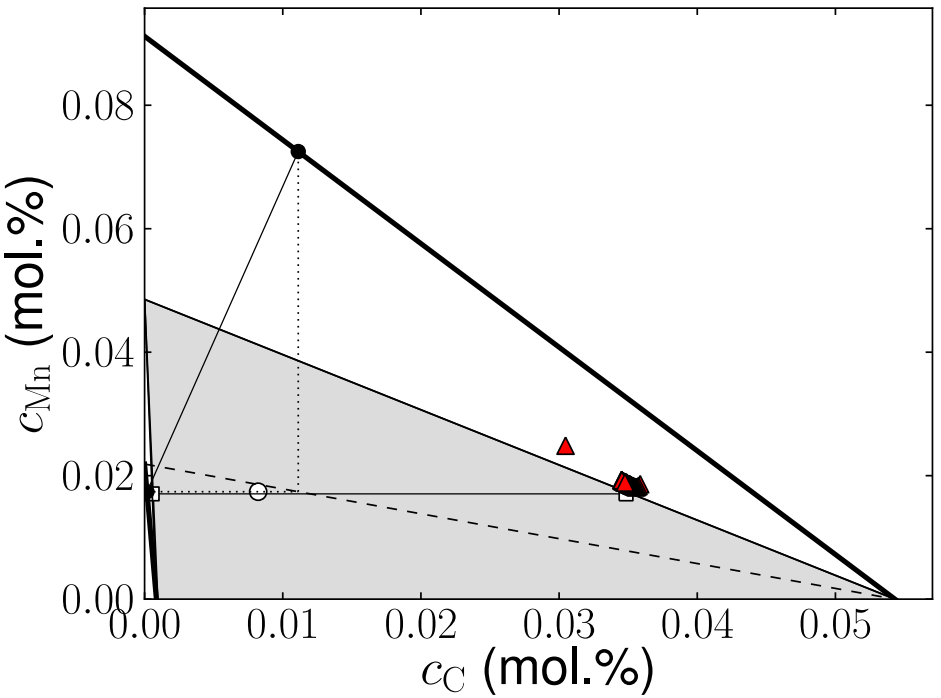
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



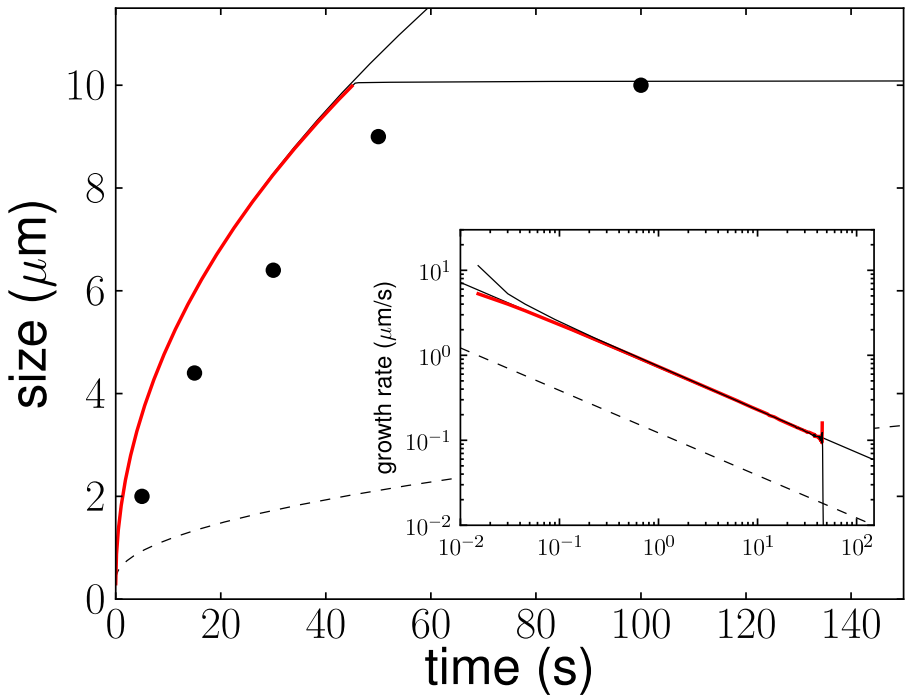


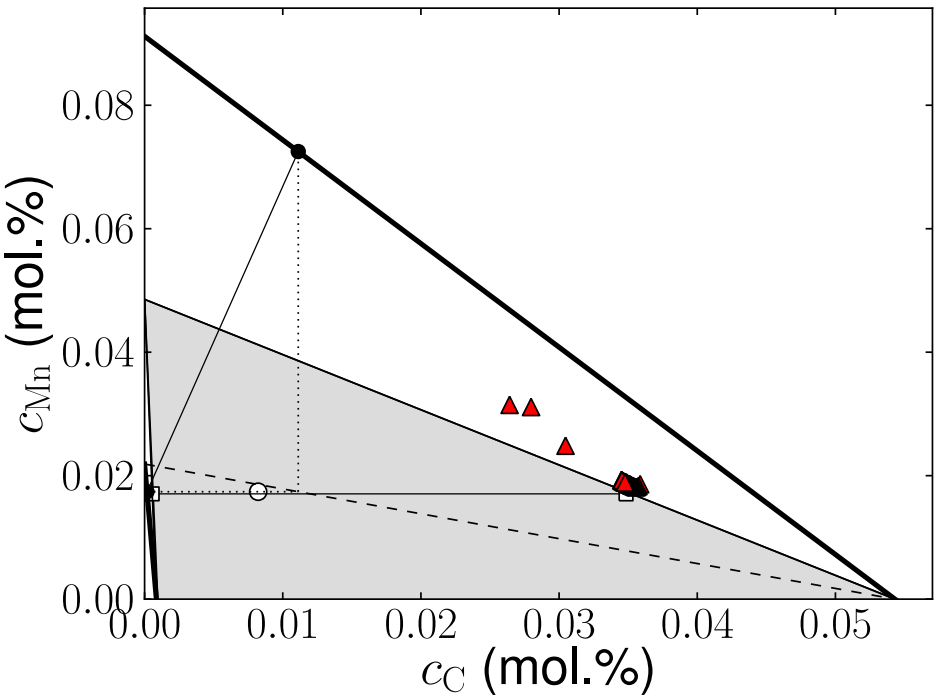
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



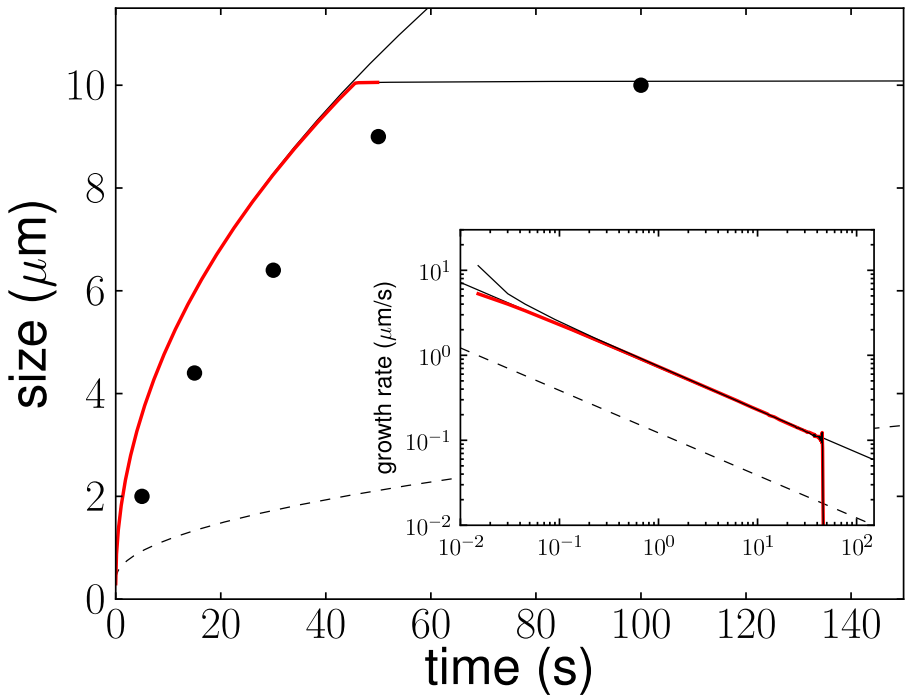


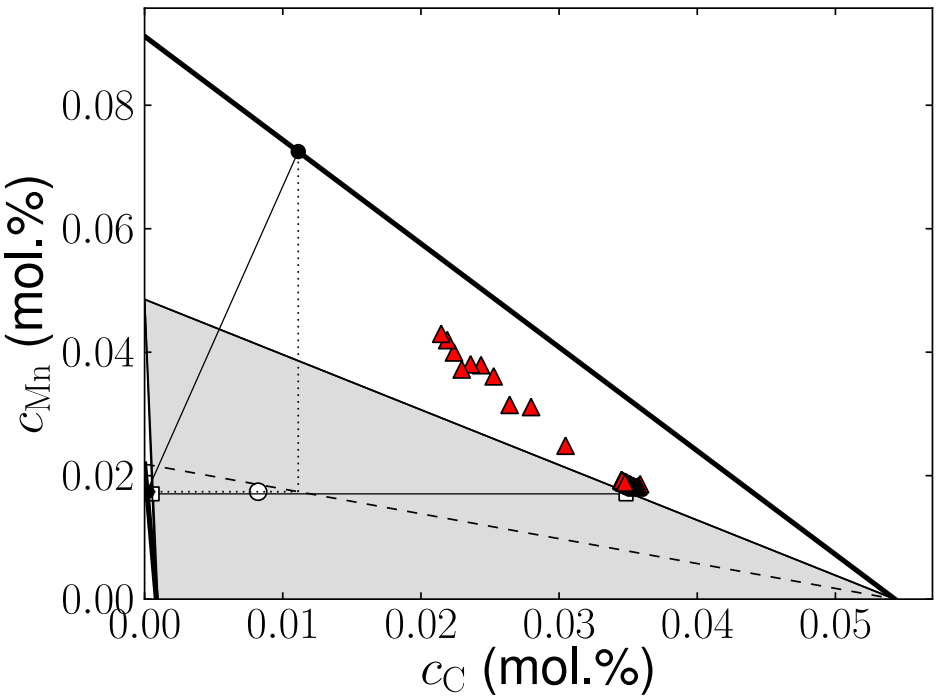
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



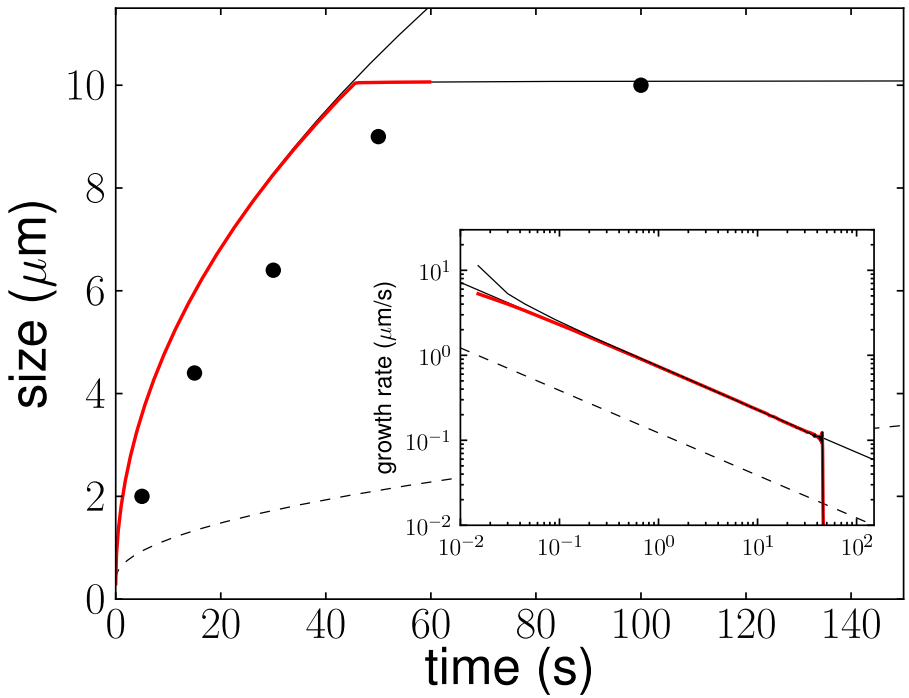


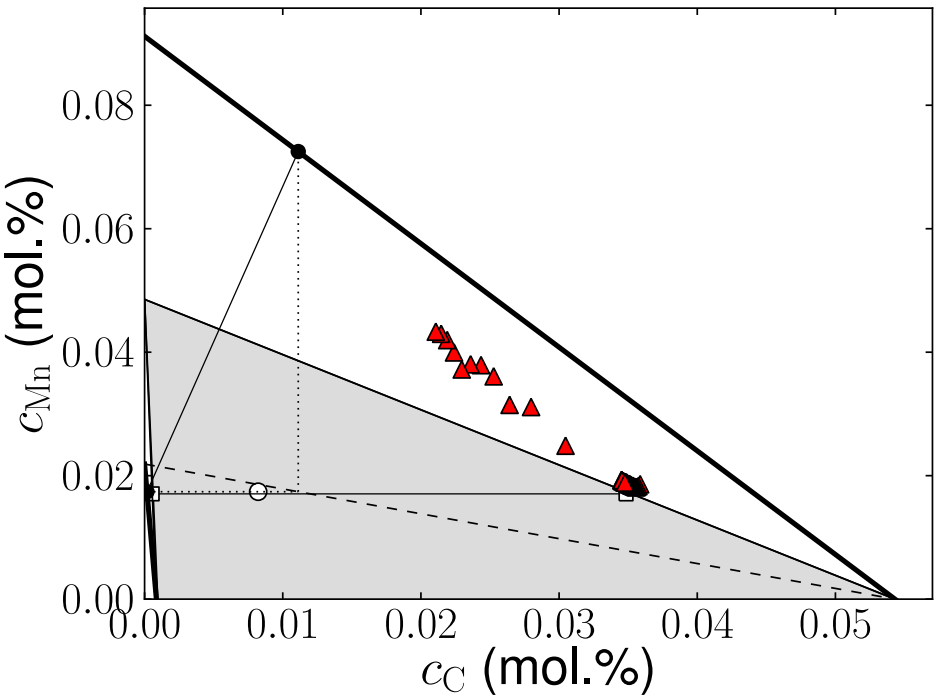
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



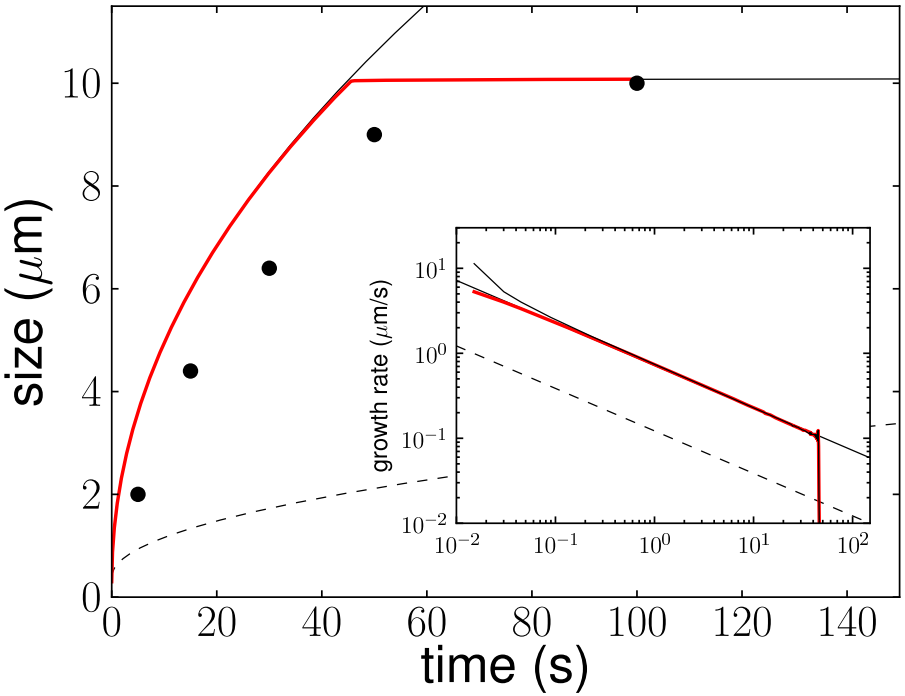


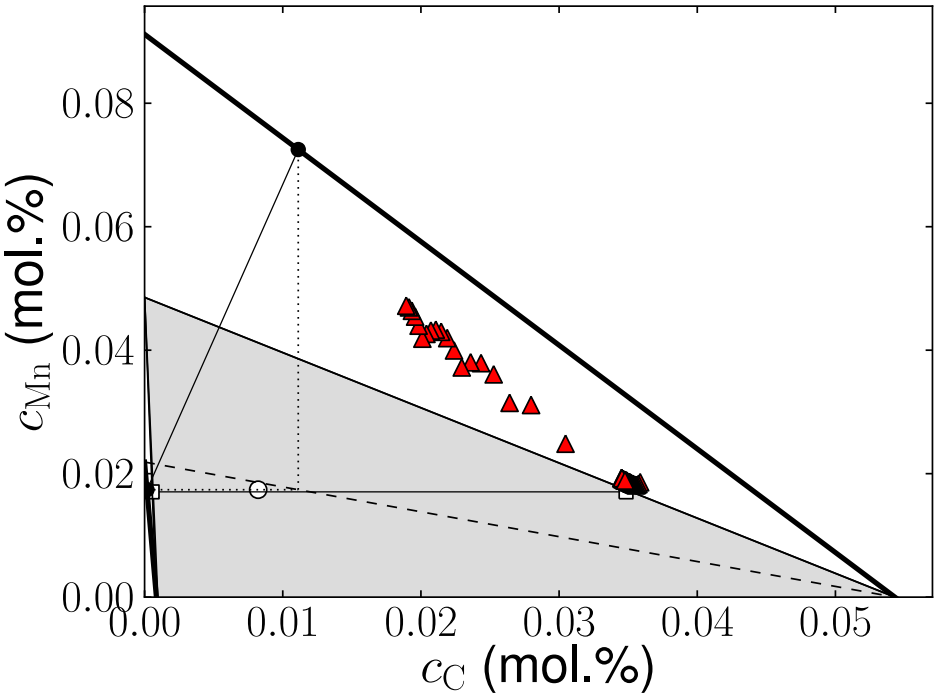
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



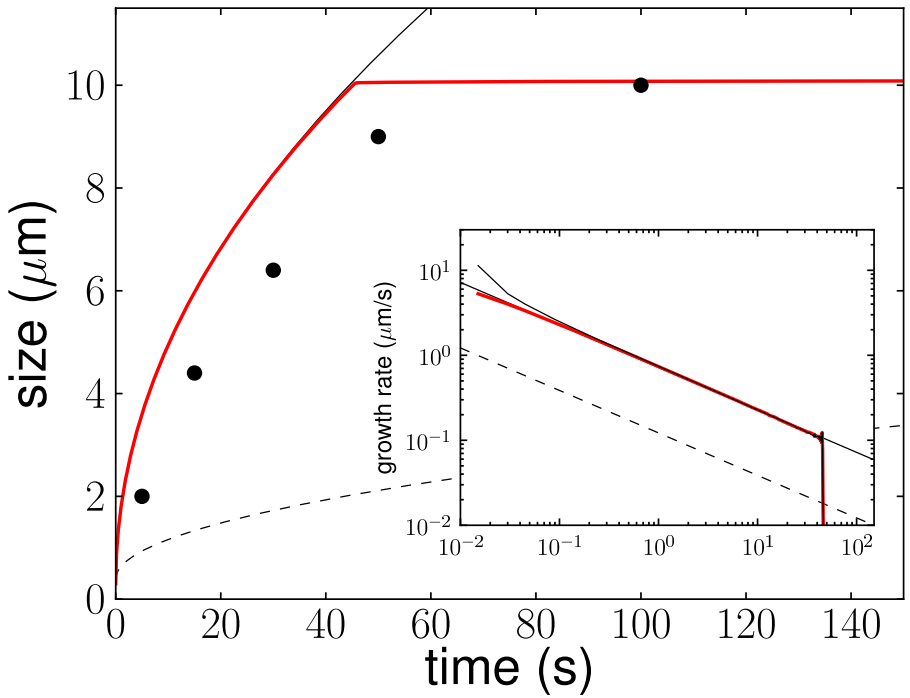


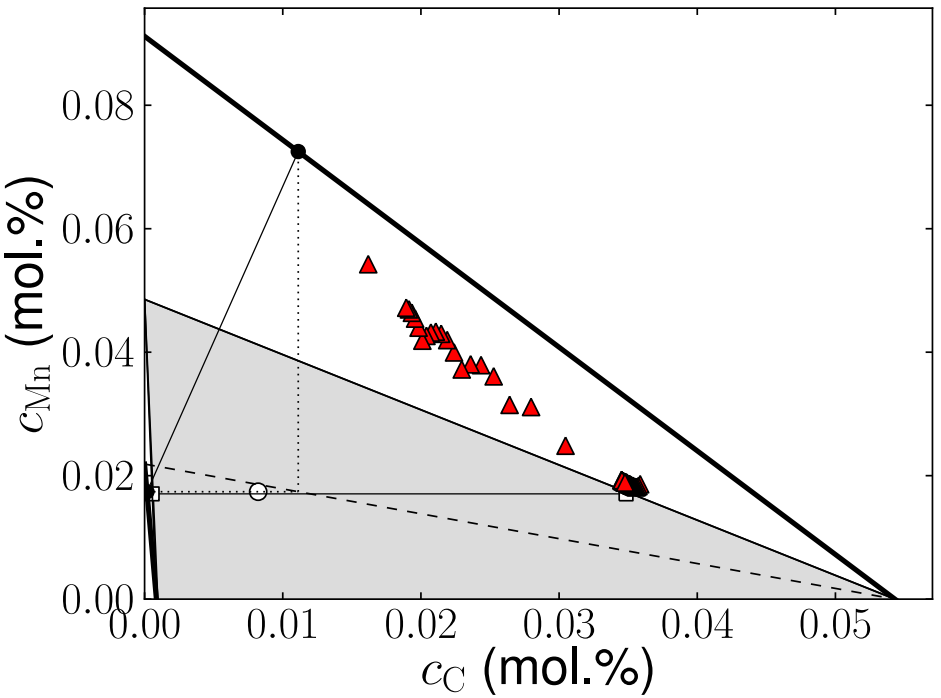
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



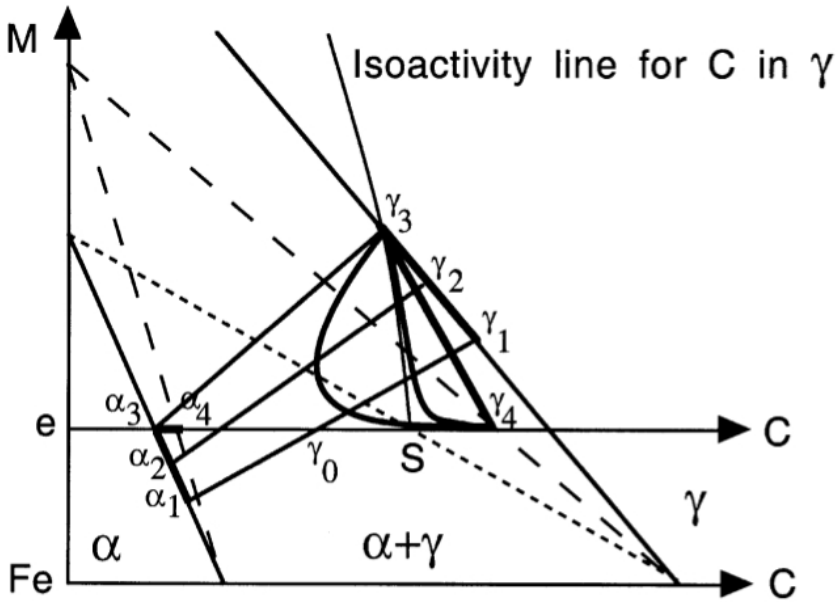


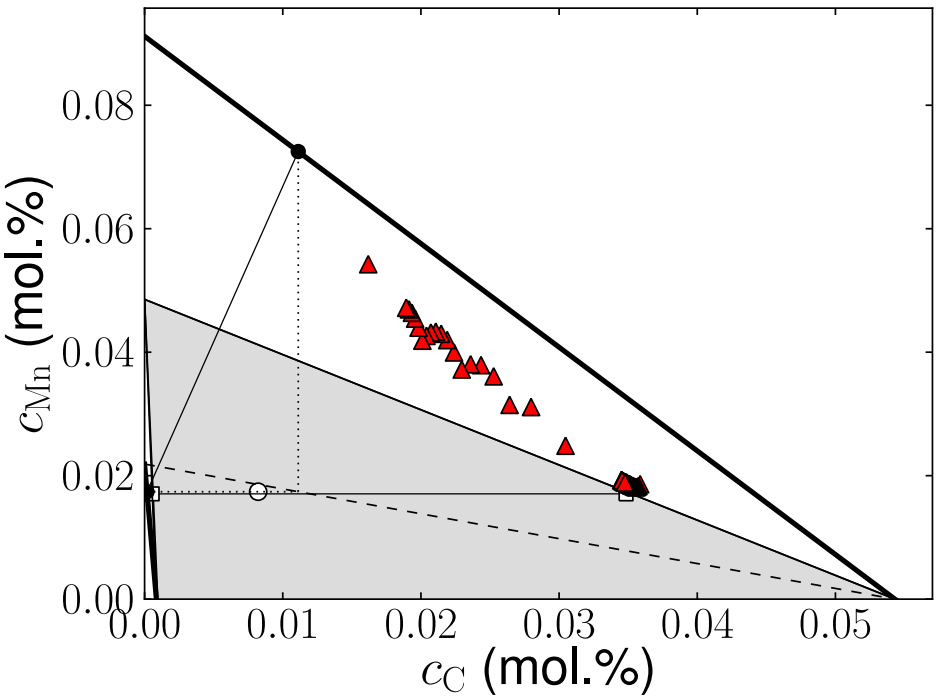
Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C





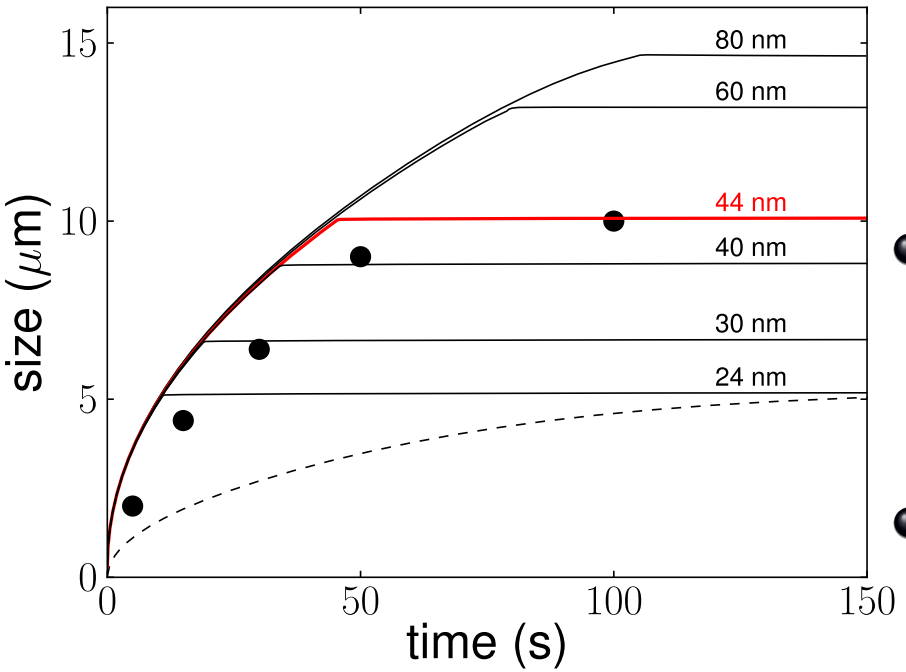
Nature of local equilibrium at the interface in the growth of ferrite from alloyed austenite [M. Hillert, Scripta Mater. 46 (2002) 447]

Growth kinetics in Fe-C-Mn

Thuillier's experiments

[Thuillier et al., Scripta Materialia 55 (2006) 1071]

- Fe – 0.08%C – 1.7%Mn; γ grain size = 20 μm; $T = 700^{\circ}$C



Influence of the interface thickness

- Weak for the first growth regime intermediate between LENP and paraequilibium (at least in 1D)
- Strong for the transition to LENP

Growth kinetics in Fe-C-Mn

Analysis of the spike

- Recasting the diffusion equation in a steady moving frame

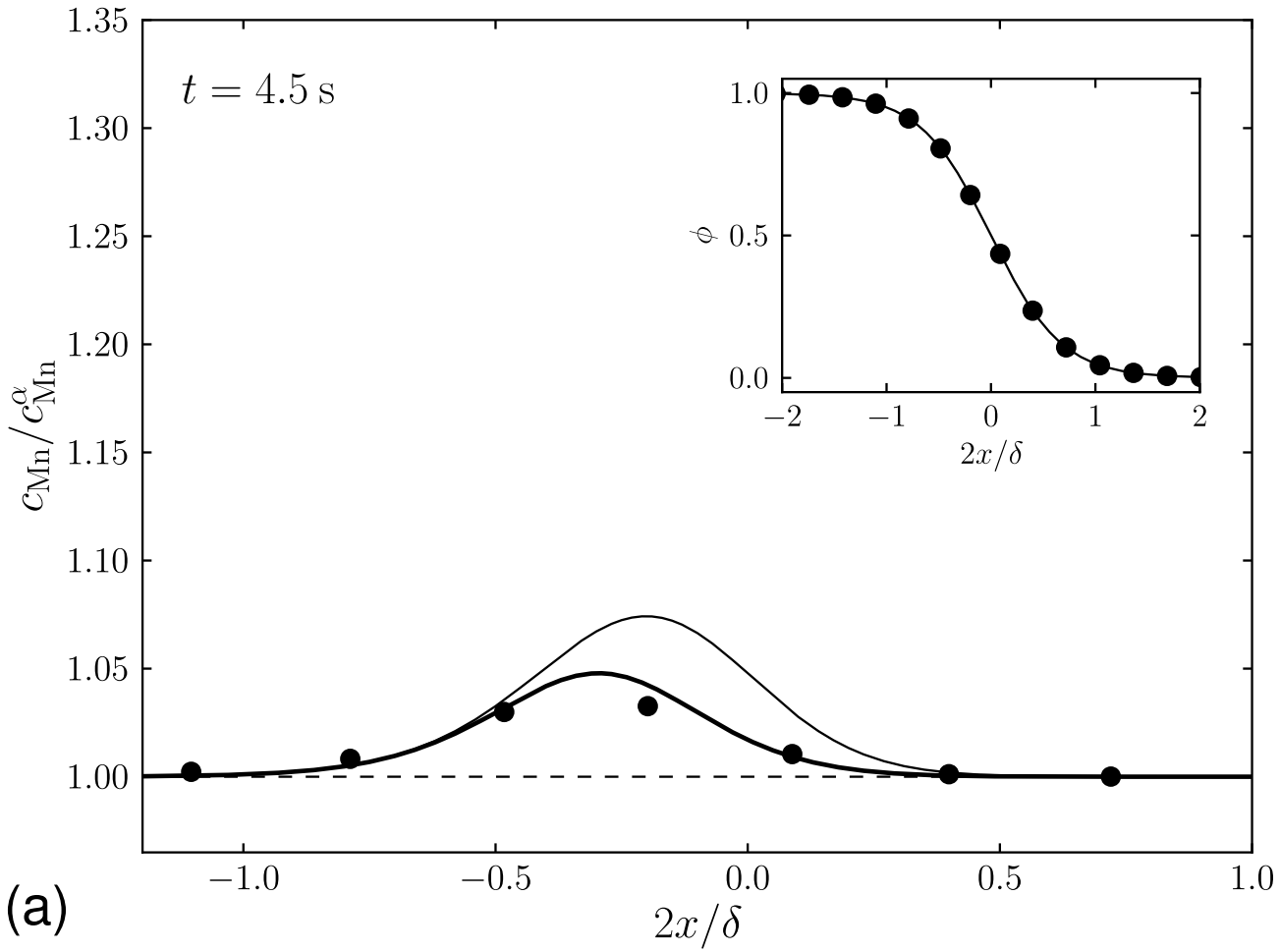
$$-v\,\mathrm{d}_x c = \mathrm{d}_x\left(L\,\mathrm{d}_x \partial_\gamma f_\gamma\right)$$

$$c^\gamma(r) = \exp(-A(r))\left[\frac{c^{\alpha*}}{k}\exp(A(-\infty)) + \int_{-\infty}^{r} \mathrm{Pe}\,B(u)\,c^{\alpha*}\exp(A(u))\,\mathrm{d}u\right]$$

where $r = 2x/\delta$, $\mathrm{Pe} = v\delta/(2D^\alpha)$

Growth kinetics in Fe-C-Mn

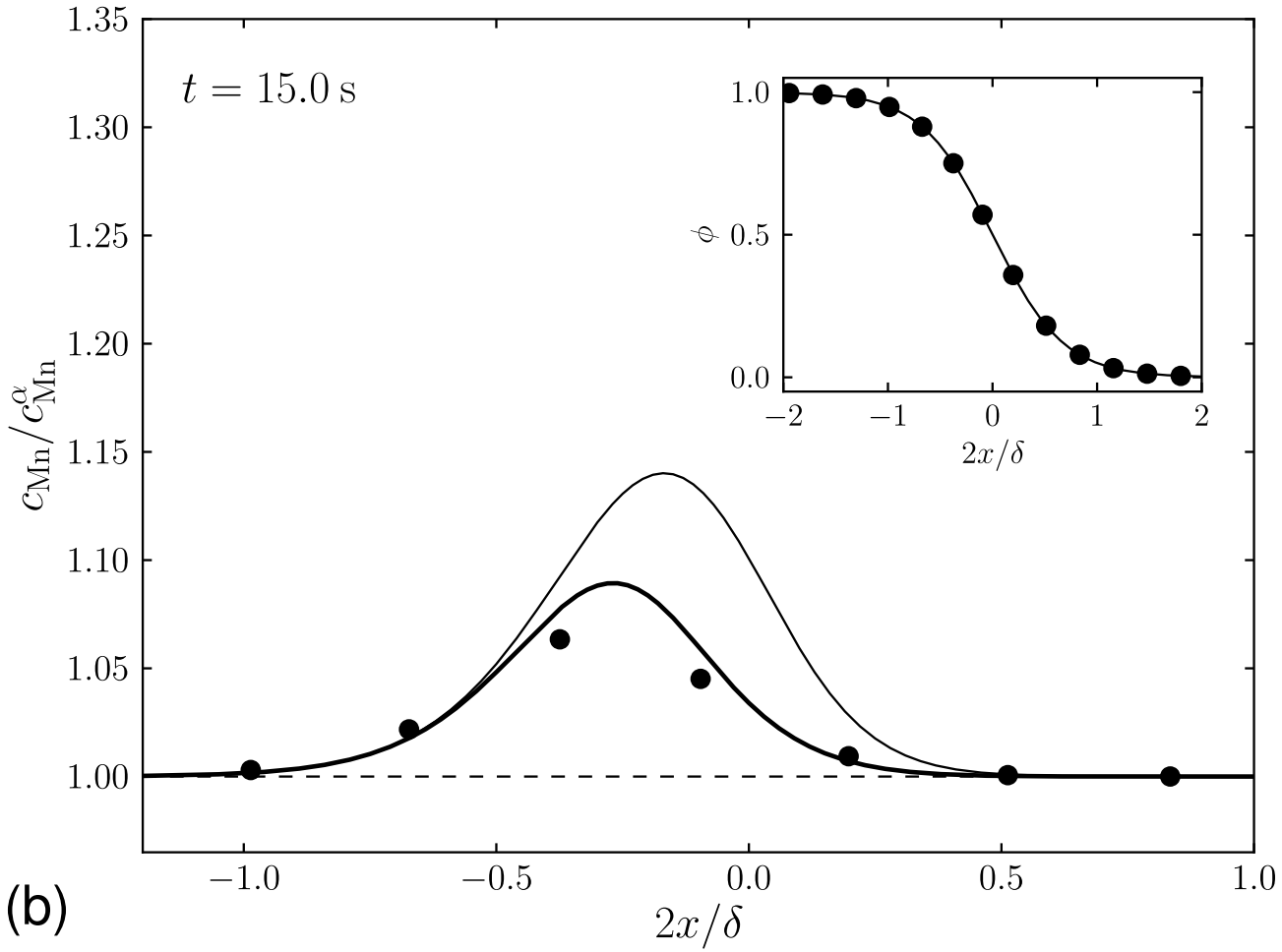
Analysis of the spike



- $L(\phi)$
- $D(\phi)$
- $D^{\alpha} = D^{\gamma}$

Growth kinetics in Fe-C-Mn

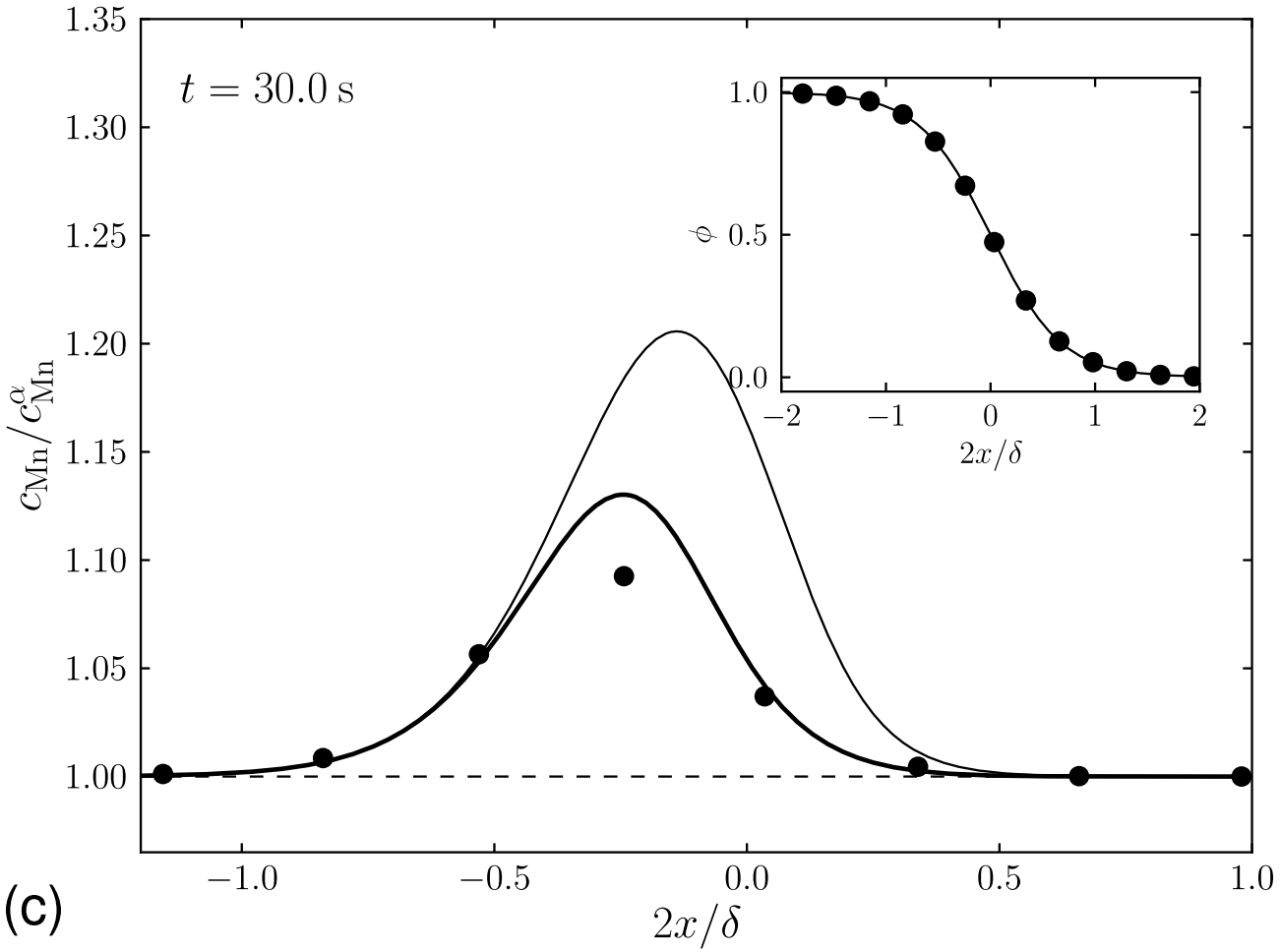
Analysis of the spike



- $L(\phi)$
- $D(\phi)$
- $D^{\alpha} = D^{\gamma}$

Growth kinetics in Fe-C-Mn

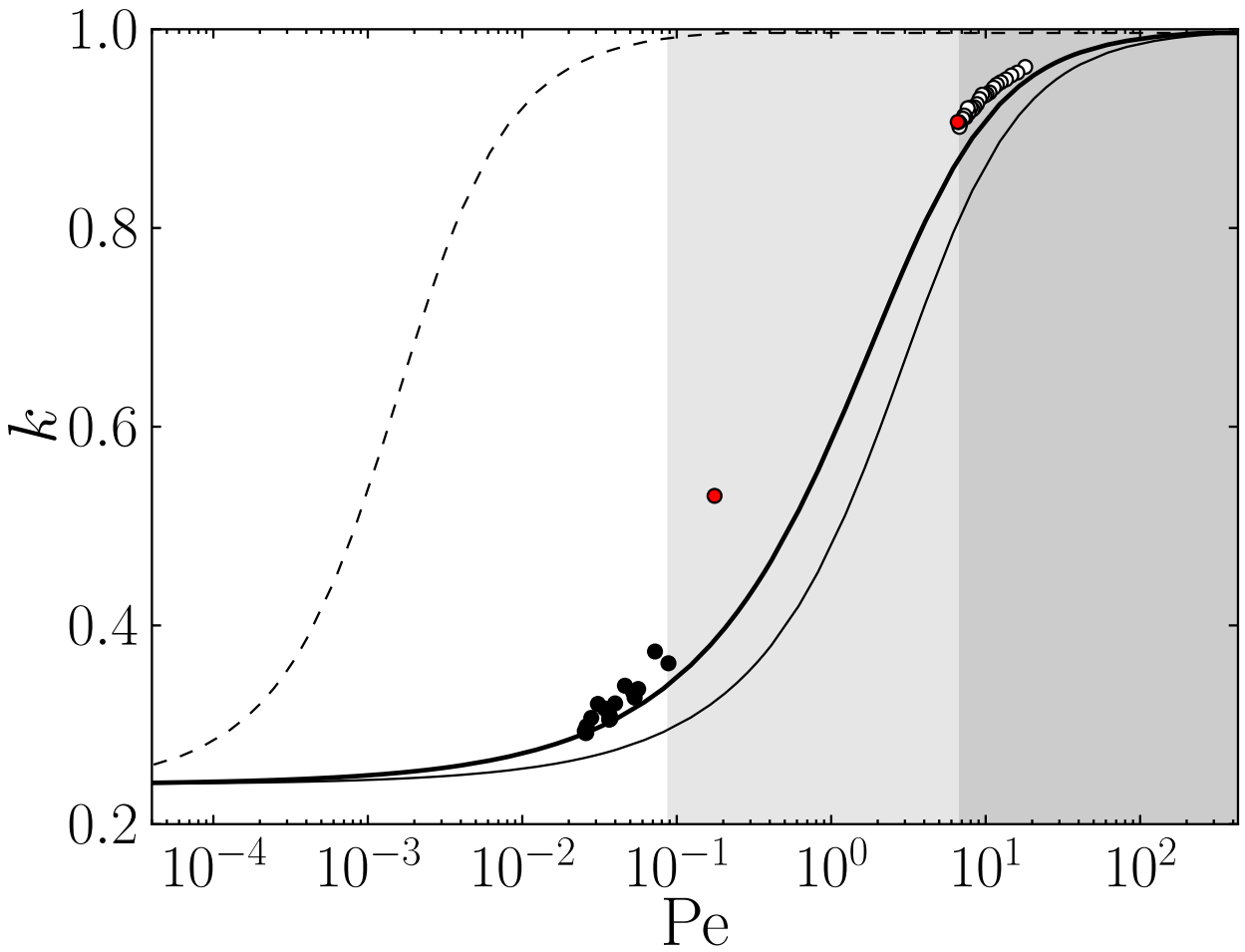
Analysis of the spike



- $L(\phi)$
- $D(\phi)$
- $D^{\alpha} = D^{\gamma}$

Growth kinetics in Fe-C-Mn

Analysis of the spike



- $L(\phi)$
- $D(\phi)$
- $D^{\alpha} = D^{\gamma}$

Growth kinetics in Fe-C-Mn

What can we conclude ?

- This is a generic behaviour (whatever δ) depending on Pe for a given interpolation of $L\,\partial_{\gamma\gamma} f_\gamma$ (the $B(u)$ effect)
- The position z_α of the *plateau* is set by a critical value Pe_t

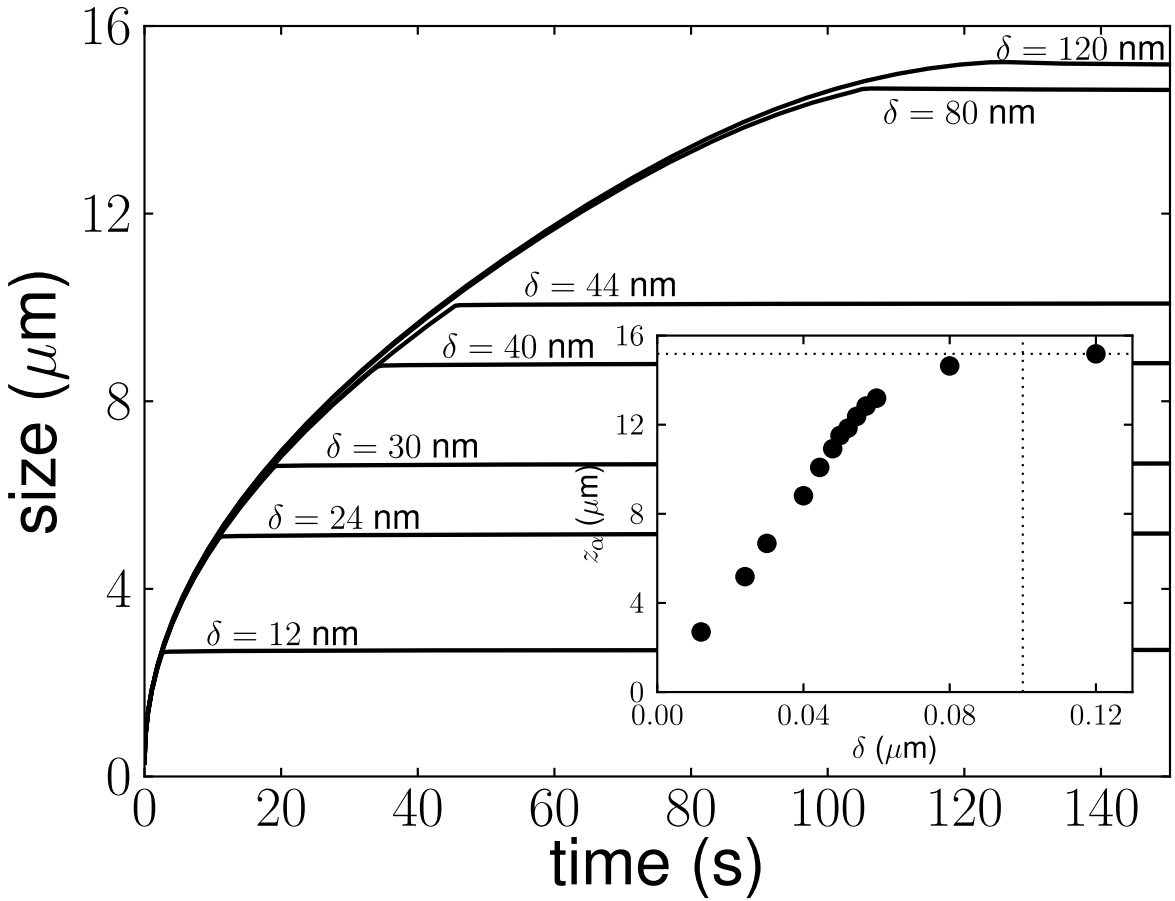
$$\Longrightarrow z_\alpha = K^2\,\delta/(4D^\alpha\,\mathrm{Pe}_t)$$

- large δ mimics slugish trans-interface Mn diffusion
  - Realistic transition for $\delta = 44$ nm
  - Realistic transition for $\delta = 12$ nm in Fe-C-Ni

  Consistent with [A. Zurob et al., Acta Mater. 56 (2008) 2203]

Growth kinetics in Fe-C-Mn

Interface versus grain size



Conclusion

9h33 in TGV this morning

- We must try to extract some interface diffusivities from our calculations
- We were not able to reproduce the trends observed in the decarburization experiments
- I'd like to play with strange interpolations of the $B(u)$ within the interface for that purpose
- and to play with cross terms in the Onsager mobility matrix