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Diffusion Simulations in CoCrFeMnNi

K. Abrahams[1], D. Gaertner[2], M. Stratmann[1], O. Shchyglo[1], S.V. Divinski[2], I. Steinbach[1]

[1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany
[2] Institute of Materials Physics, University of Münster, Germany

INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

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Until last meeting…

- Big question: Sluggish diffusion in HEAs ???

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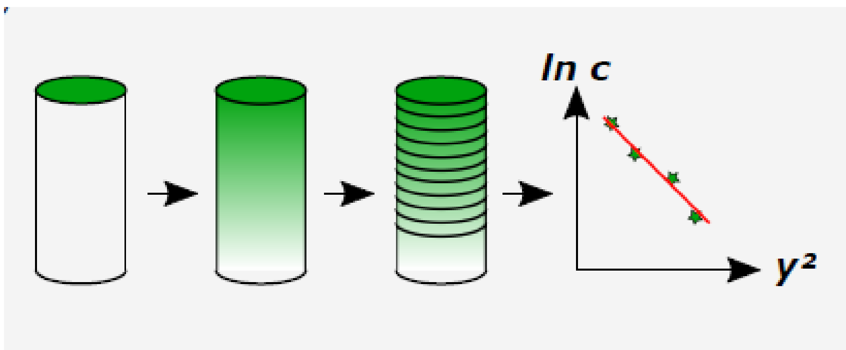
- **Tracer diffusion measurements and simulations in equiatomic CoCrFeMnNi**

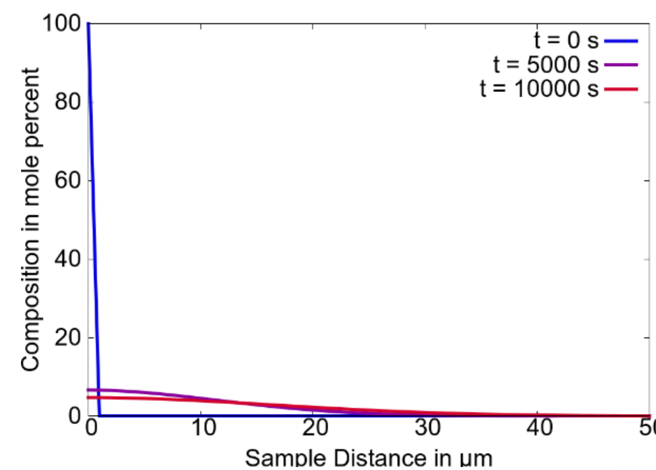
Tracer diffusion

Tracer: radioactive isotopes



100 at% Ni* | 100 at% Ni

Ni tracer profile



Distinguish tracer and „normal " atoms

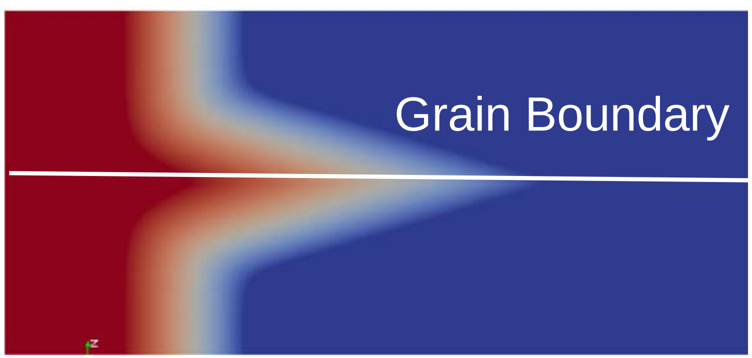
$$\frac{\partial c_{A^*}}{\partial t} = D_{A^*}(c)\,\frac{\partial^2 c_{A^*}}{\partial x^2}$$

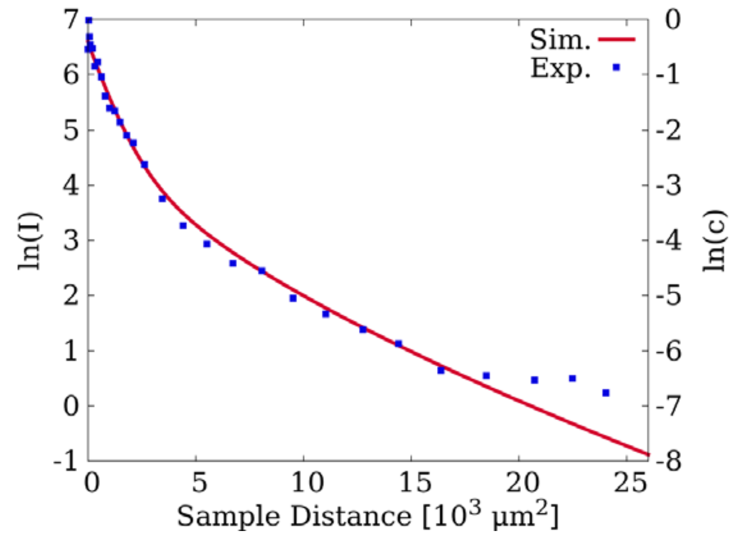
$$D_{A^*}(c) = RTM_A(c)$$

- Big question: Sluggish diffusion in HEAs ???
- **Tracer diffusion measurements and simulations in equiatomic CoCrFeMnNi**

Initial

Final





→ Diffusion of one element in one alloy at one temperature

Until last meeting…

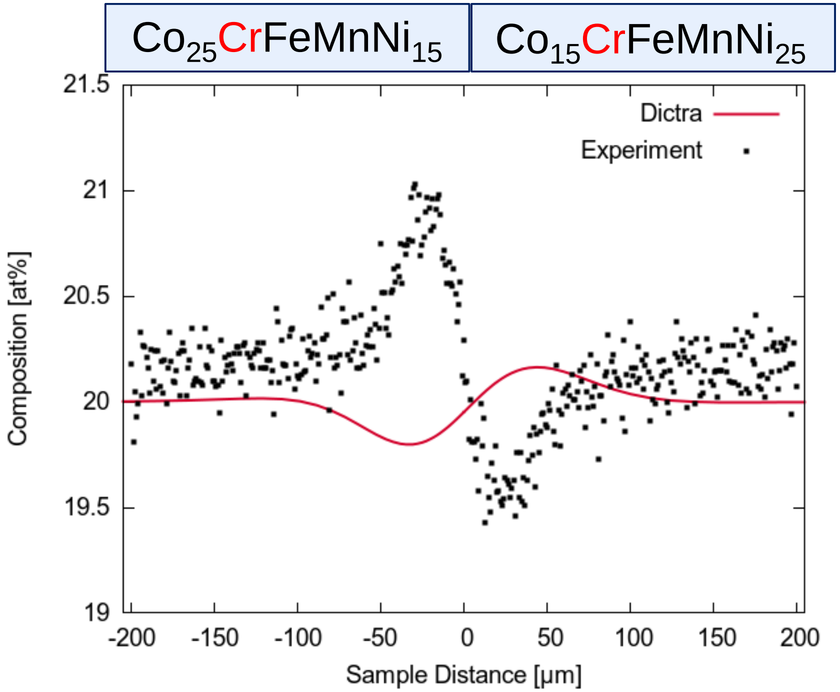
- Big question: Sluggish diffusion in HEAs ???
- Tracer diffusion measurements and simulations in equiatomic CoCrFeMnNi
- **Diffusion Couple measurements and simulations**

Multicomponent diffusion model: DICTRA model

→ Physical meaning ?

→ Applicability in high concentrated multicomponent alloys?

→ Simplifications (e.g. No kinetic cross terms, reference elements)



Possible reasons:

- Thermodynamic database?
- Kinetic database?
- Diffusion model?

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Possible reasons

- Thermodynamic database?
- Kinetic database?
- Diffusion model?

… and then?

New from the simulation side: **Generalized diffusion model**

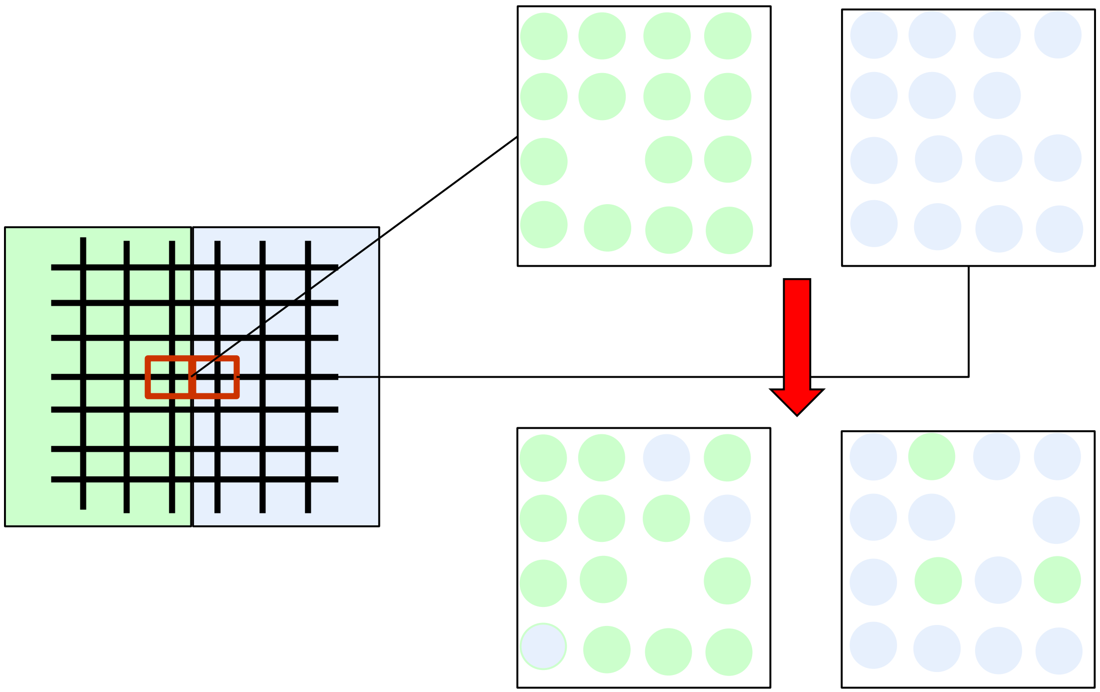
Pair-diffusion model

- pair-wise interactions

$$\frac{\partial x_i}{\partial t} = \frac{1}{2} \nabla \sum_{\substack{j=1 \\ j \neq i}}^{n} x_i x_j M_{ij} \nabla \tilde{\mu}_{ij}$$

kinetic

thermodynamic



- Vacancies in equilibrium

Pair-diffusion model

Derivation:

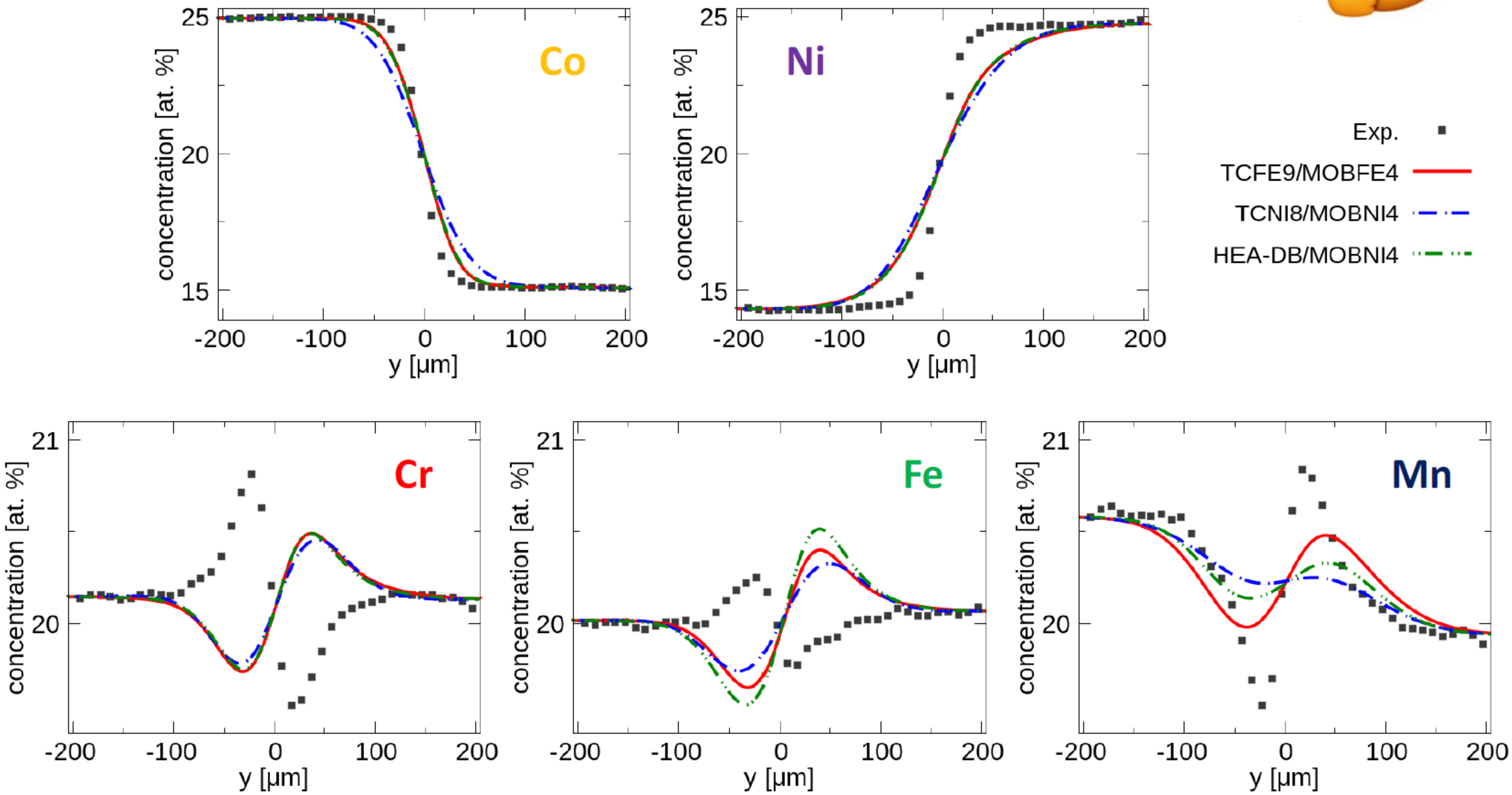
- Mass conservation equation: $\frac{\partial x_i}{\partial t} + \nabla J_i + \nabla(x_i v) = 0$
- Velocity: $\nabla v = -\sum_{j=1}^{n} \nabla J_j V_j$
- Intrinsic flux: $J_i = -M_i x_i \nabla \mu_i$

$$\frac{\partial \boldsymbol{x}_i}{\partial t} = \frac{1}{2} \nabla \sum_{\substack{j=1 \\ j \neq i}}^{n} \boldsymbol{x}_i \boldsymbol{x}_j \boldsymbol{M}_{ij} \nabla \tilde{\boldsymbol{\mu}}_{ij}$$

$$\tilde{\boldsymbol{\mu}}_{ij} = \boldsymbol{\mu}_i - \boldsymbol{\mu}_j$$

$$\boldsymbol{M}_{ij} = \boldsymbol{x}_i \boldsymbol{M}_j + \boldsymbol{x}_j \boldsymbol{M}_i + \sum_{\substack{k=1 \\ k \neq i \\ k \neq j}}^{n} \boldsymbol{x}_k \left(\boldsymbol{M}_i + \boldsymbol{M}_j - \boldsymbol{M}_k\right)$$

Interdiffusion: New diffusion model

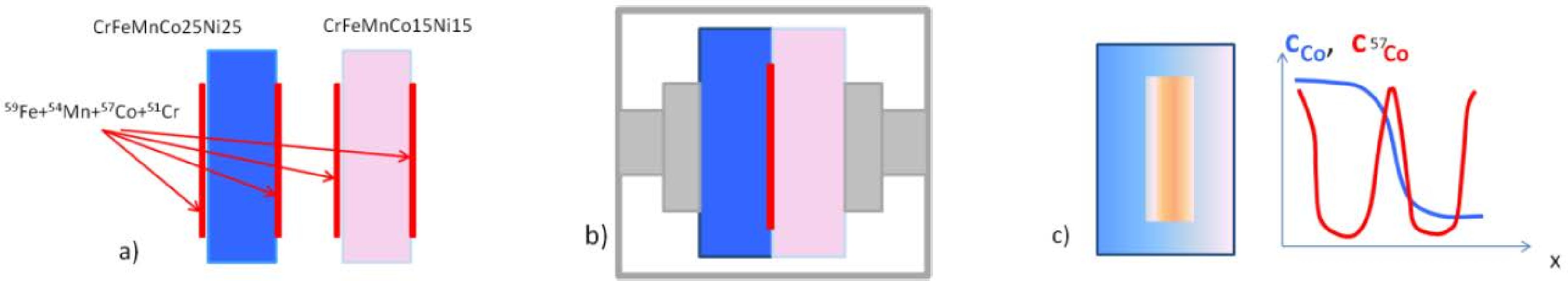


Possible reasons

- Thermodynamic database?
- Kinetic database?
- ~~Diffusion model?~~

… and then?

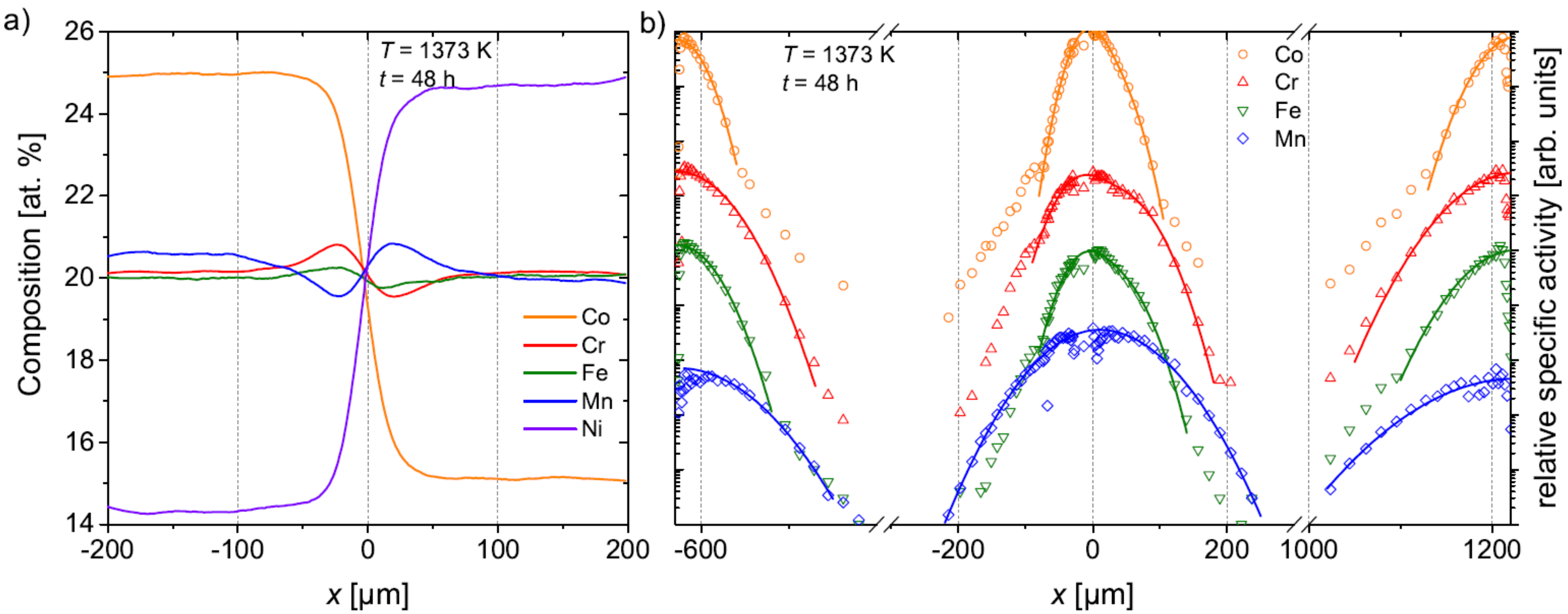
New from the experimental side: **Combined radiotracer and interdiffusion experiment**



→ Composition dependent atomic mobilities from one experiment!

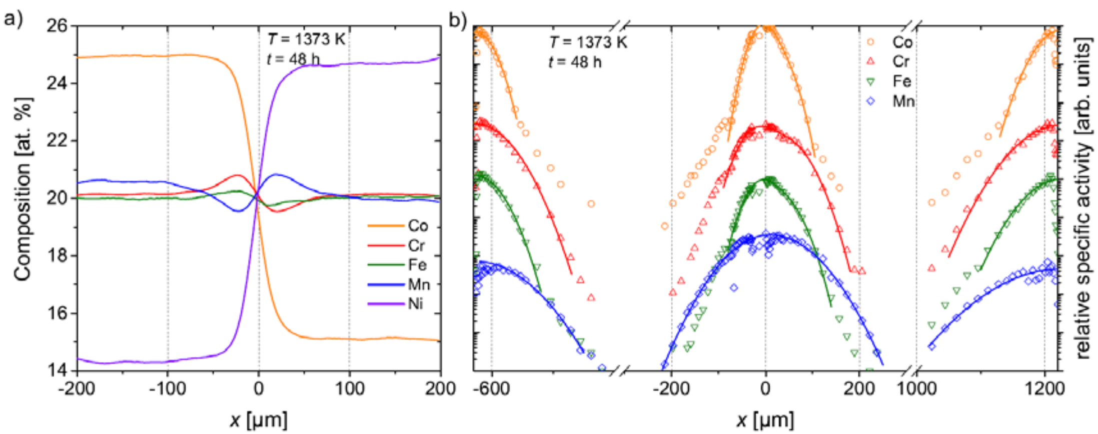
[1] I.V. Belova, N.S. Kulkarni, Y.H. Sohn, G.E. Murch: Simultaneous measurement of tracer and interdiffusion coefficients: an isotopic phenomenological diffusion formalism for the binary alloy (2013)
[2] I.V. Belova, N.S. Kulkarni, Y.H. Sohn, G.E. Murch: Simultaneous tracer diffusion and interdiffusion in a sandwich-type configuration to provide the composition dependence of the tracer diffusion coefficients (2014)
[3] I.V. Belova,Y.H. Sohn, G.E. Murch: Measurement of tracer diffusion coefficients in an interdiffusion context for multicomponent alloys (2015)

Combined radiotracer and interdiffusion experiment



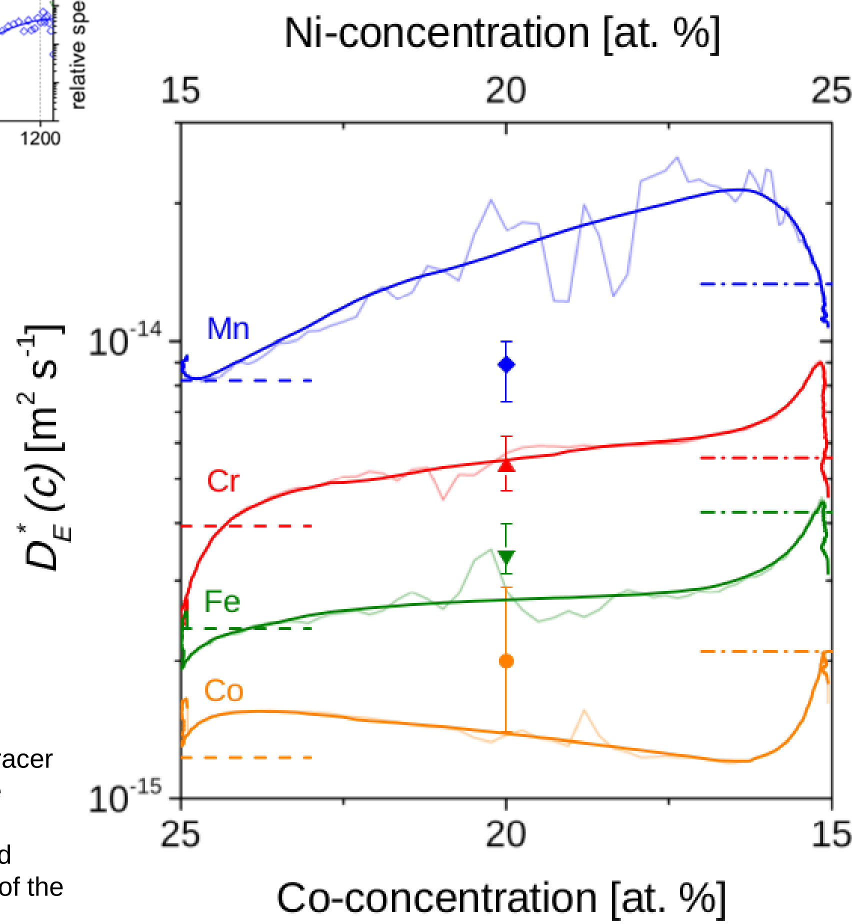
Composition dependent atomic mobilities!!!

$Co_{25}CrFeMn$ Ni_{15}	$Co_{15}CrFeMn$ Ni_{25}



Thin layer isotope sandwich configuration from Belova and Murch

$$D_A^*(c) = -\left(\frac{(x+a)}{2t} - \frac{G_A(x)}{c_A(x)}\right) / \left(\frac{\partial lnc_A^*}{\partial x} - \frac{\partial lnc_A(x)}{\partial x}\right)$$



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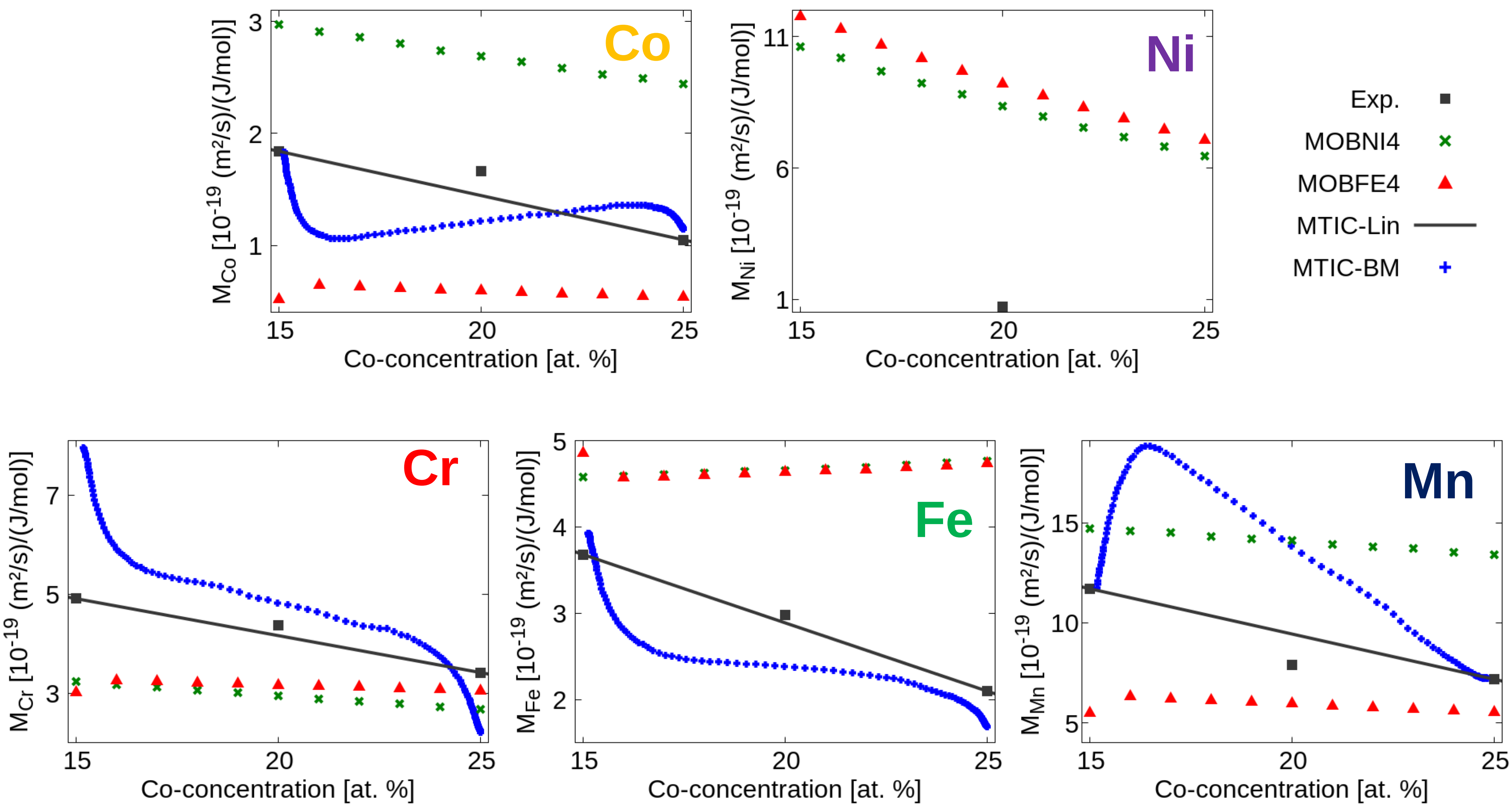
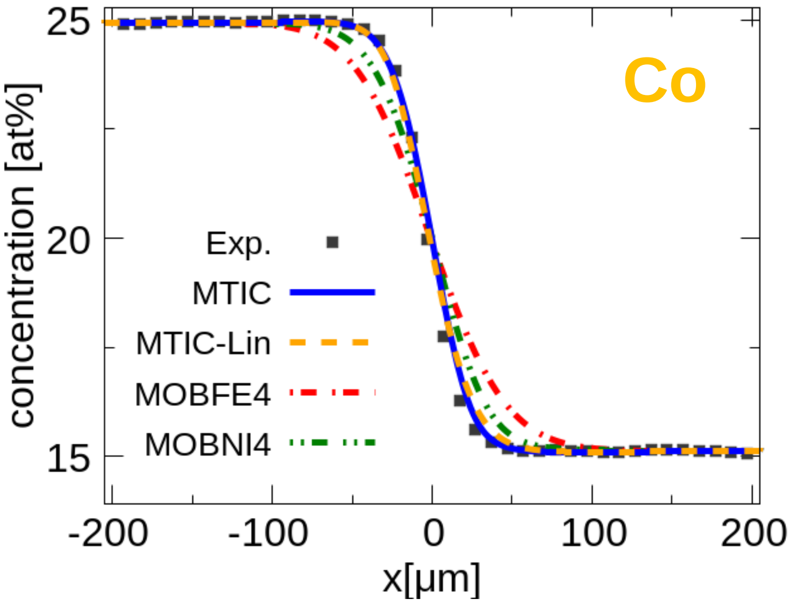
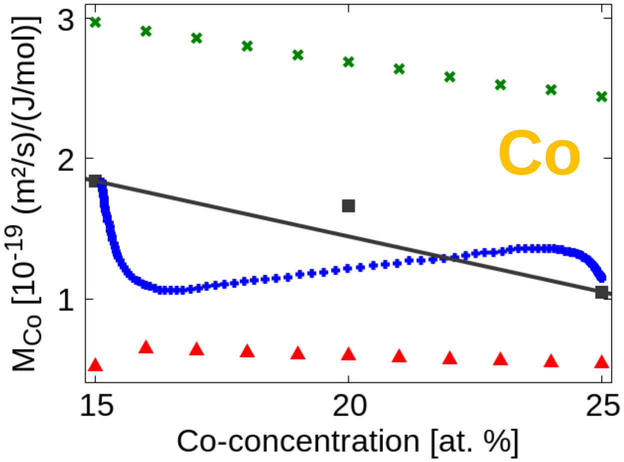
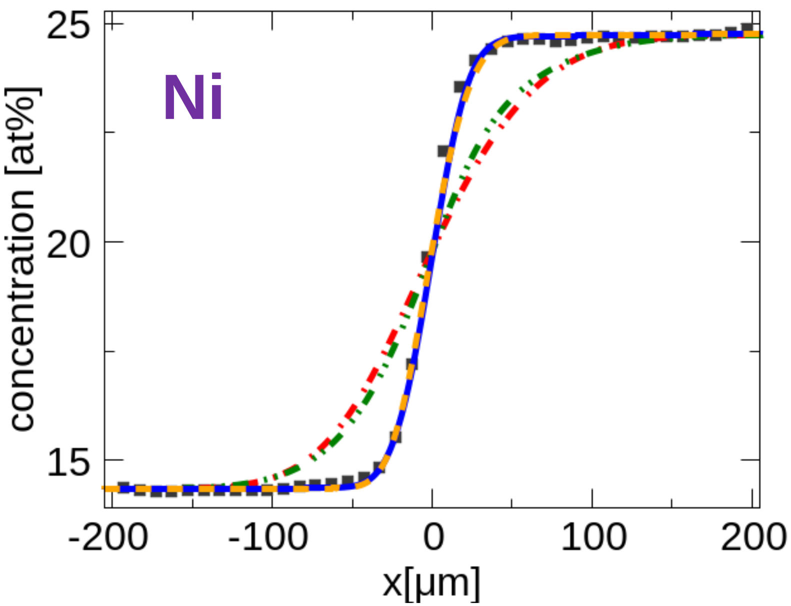
Comparison Atomic Mobilities

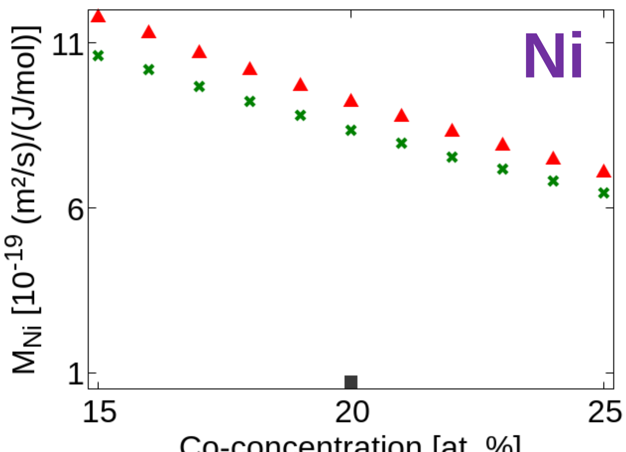


Interdiffusion Co and Ni

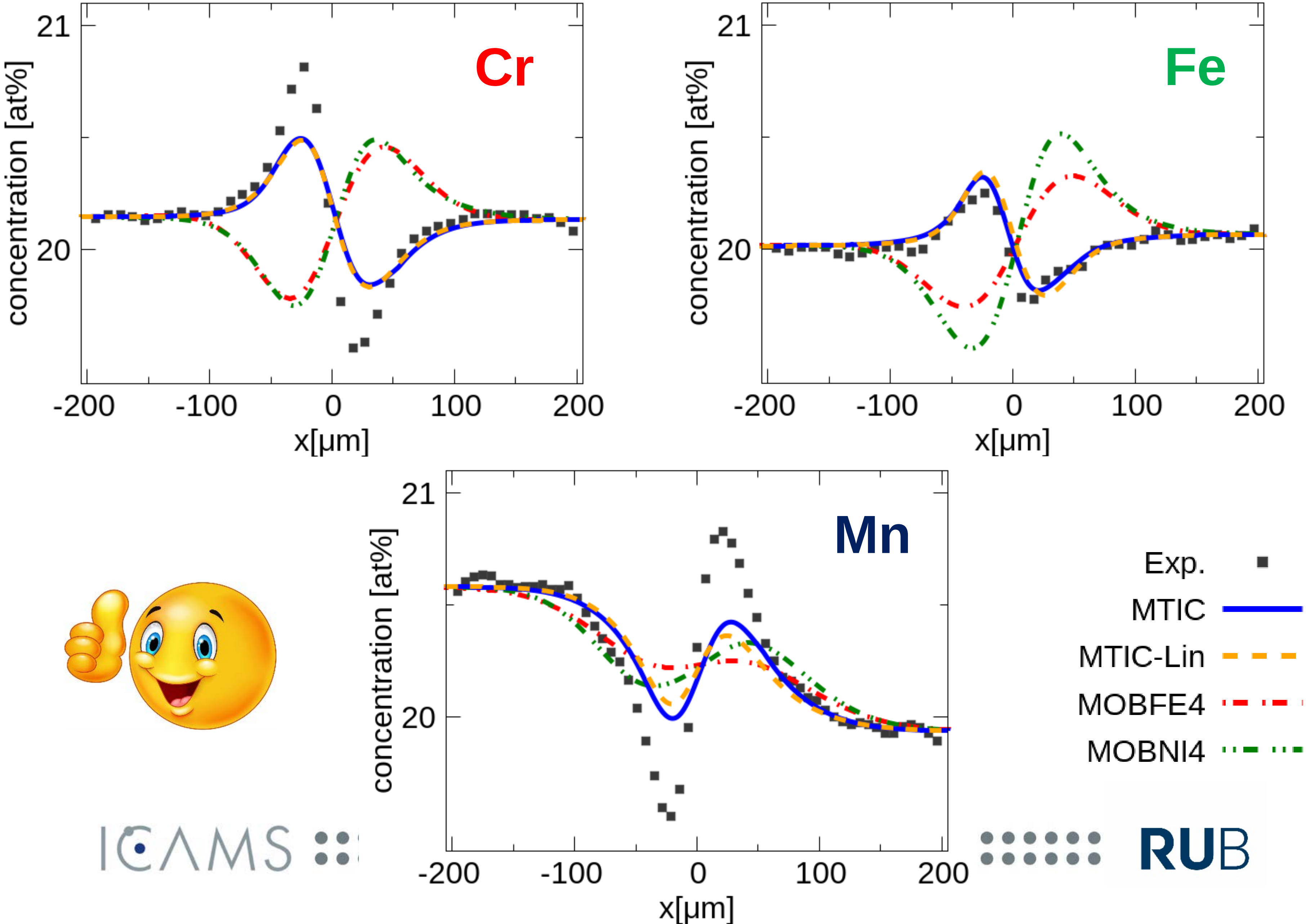




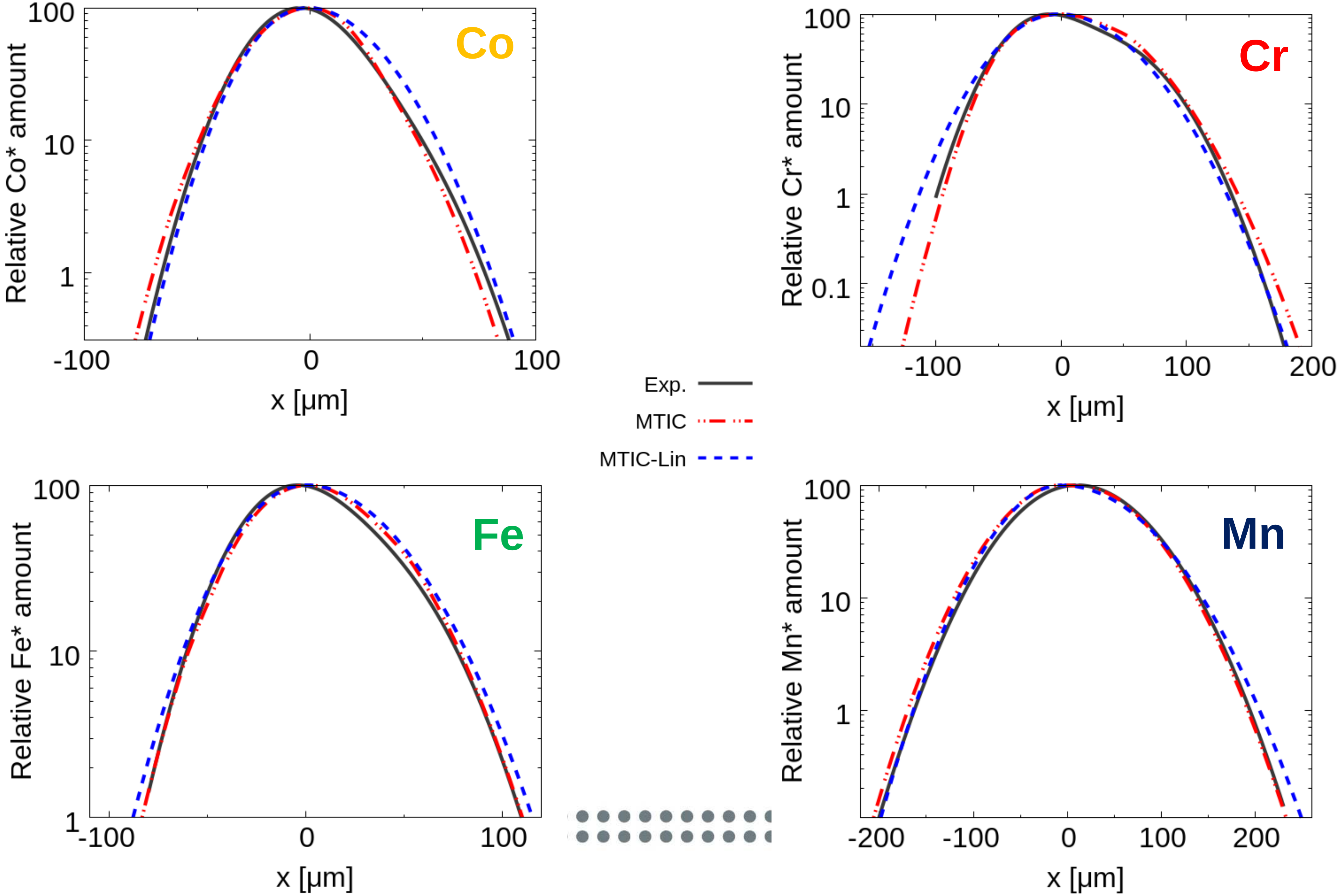




Interdiffusion Cr, Fe, Mn



Tracer diffusion profiles



Summary and Outlook

- Accurate kinetics are important!

- Further testing of the method to determine composition dependent atomic mobilities

- Extend diffusion model to more than one sublattice and to intersticial elements

- Assessment of atomic mobility data for the new model

- Automate the assessment of atomic mobility data