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Diffusion Simulations in High-Entropy Alloys

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Why diffusion simulations ?

- Homogenization heat treatment

- Important for microstructural evolution
  - → Nucleation and phase growth sensitive to local concentration
  - → Phase stability

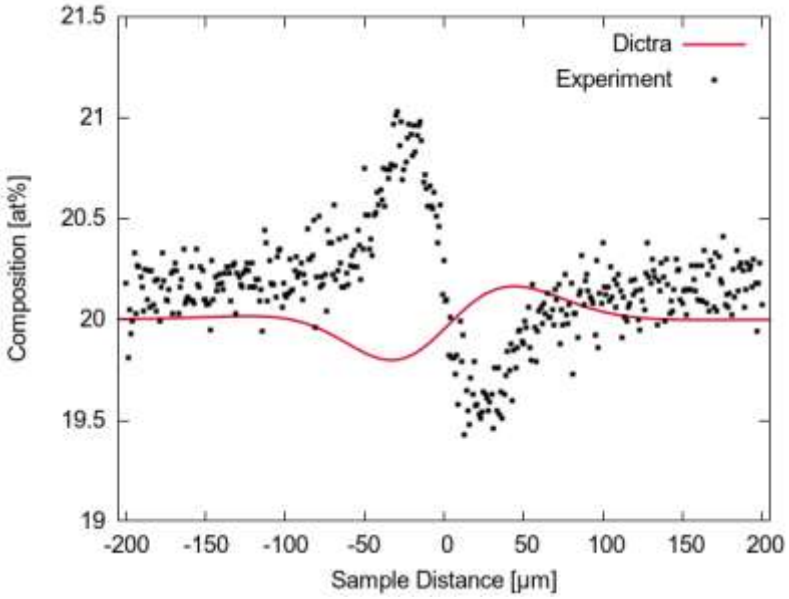
- Understand diffusion mechanism
  - → dilute limit ↔ high concentrated alloy
  - → coupling of thermodynamic and kinetics
  - → influence of thermodynamic/kinetic cross terms

- Validate databases
  - → kinetic databases (tracer diffusion experiments, interdiffusion experiments)
  - → thermodynamic database (interdiffusion experiment)

Diffusion Simulations: State of the art

- Multicomponent diffusion model: DICTRA model
  - → applicability in high concentrated multicomponent alloys
  - → simplifications (e.g. No kinetic cross terms, reference elements)
  - → kinetic databases fitted to this model

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



- No combination with self-diffusion model

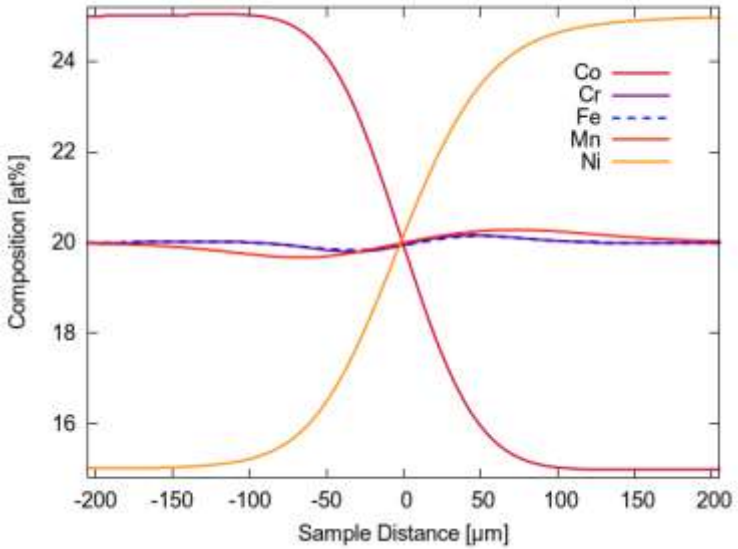
New simulation methods

Interdiffusion

$$\frac{\partial y_i}{\partial t} = \nabla \sum_{j=1, j\neq i}^{n} M_{ij} \nabla \tilde{\mu}_{ij}$$

kinetic thermodynamic

- pair-wise interactions



Tracer-/Self-diffusion

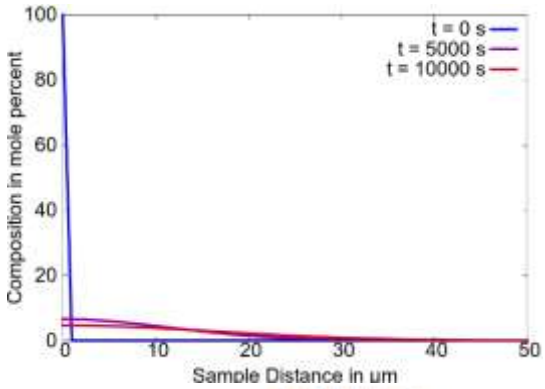
Distinguish tracer and „normal “ atoms

$$\frac{\partial c_{A^*}}{\partial t} = D_{A^*} \frac{\partial^2 c_{A^*}}{\partial x^2}$$

$$D_{A^*} = RTM_A$$

100 at% Ni* | 100 at% Ni

Ni tracer profile

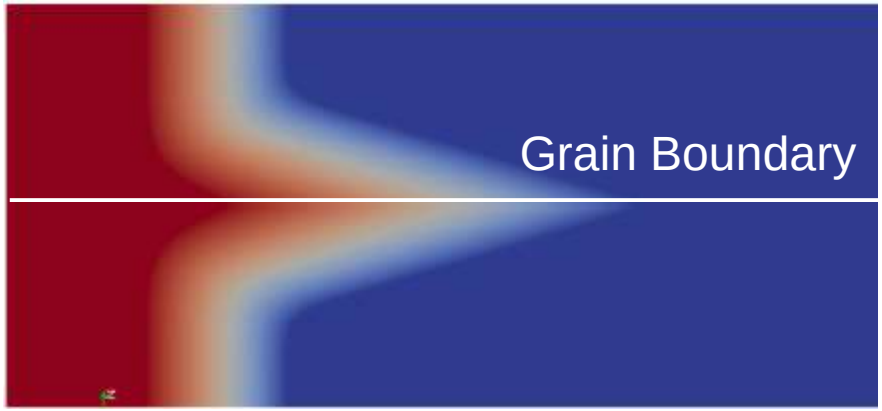


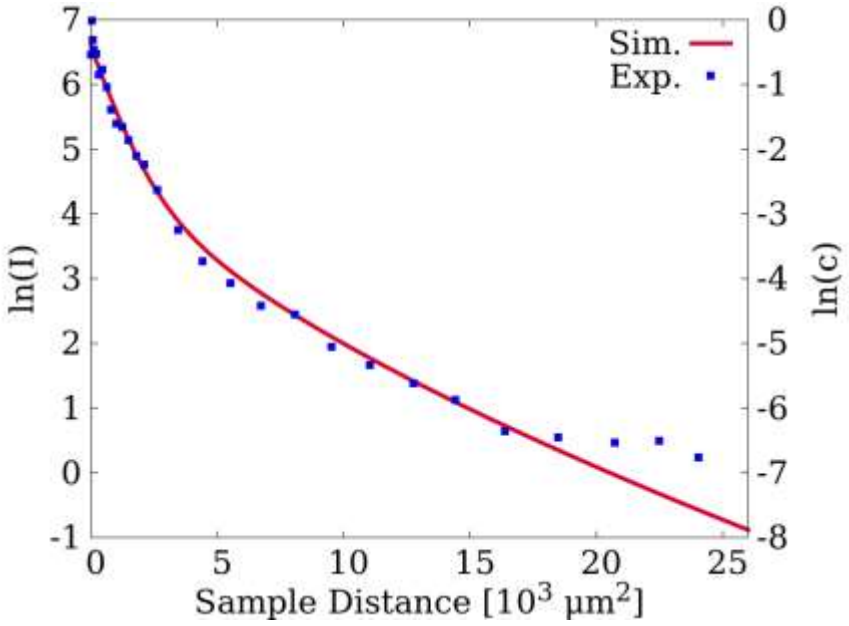
New simulation methods

Faster diffusion on GBs

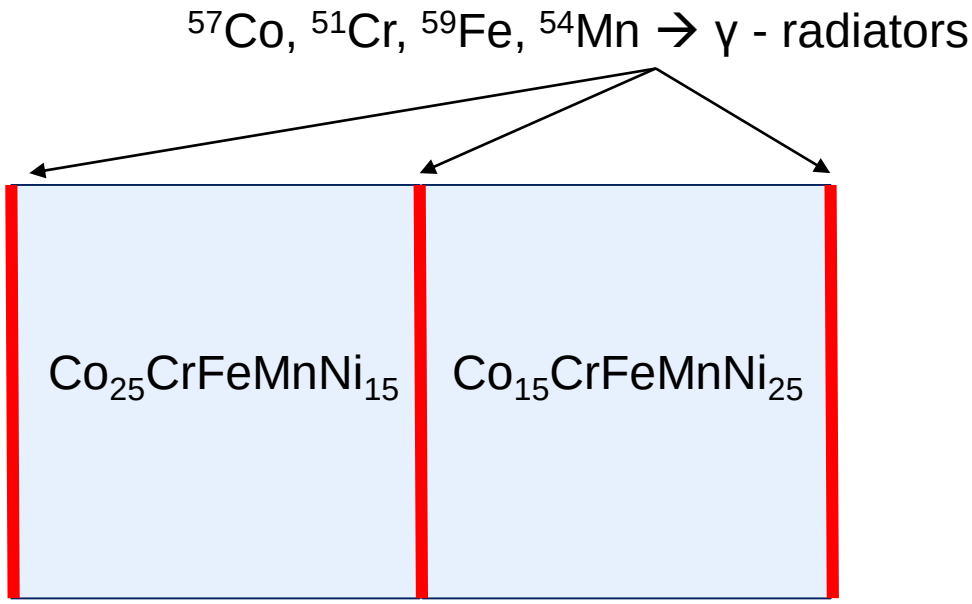
Initial

Final





Example CoCrFeMnNi



Annealing time: 48 h

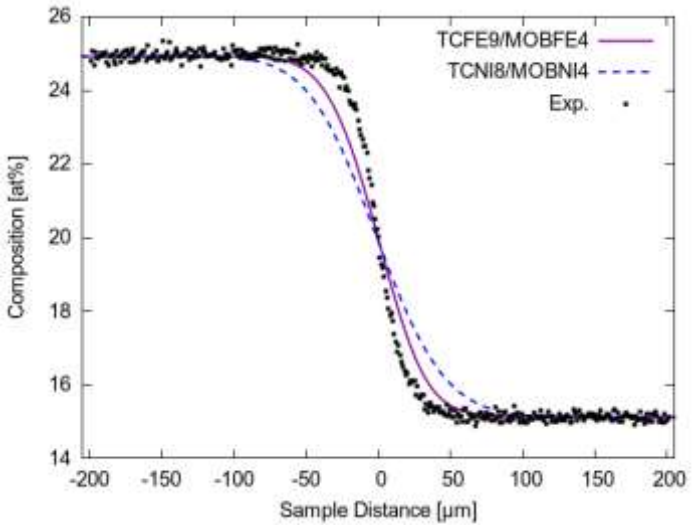
Annealing temperature 1373 K

Polycrystalline material

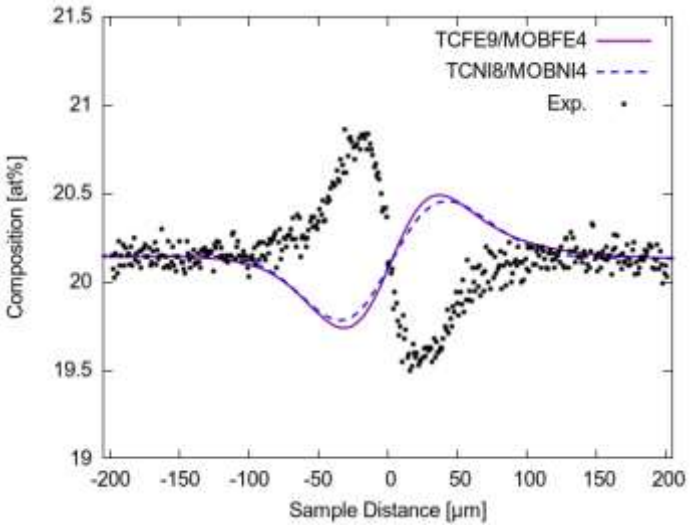
Example CoCrFeMnNi: Interdiffusion

$Co_{25}CrFeMnNi_{15}$	$Co_{15}CrFeMnNi_{25}$

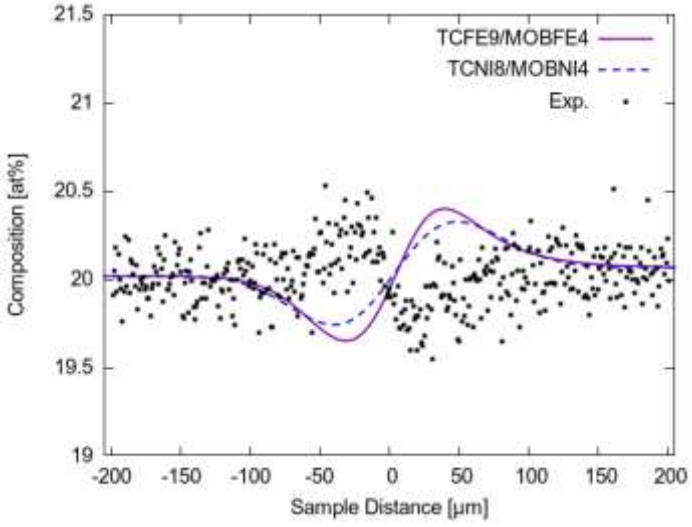
Co



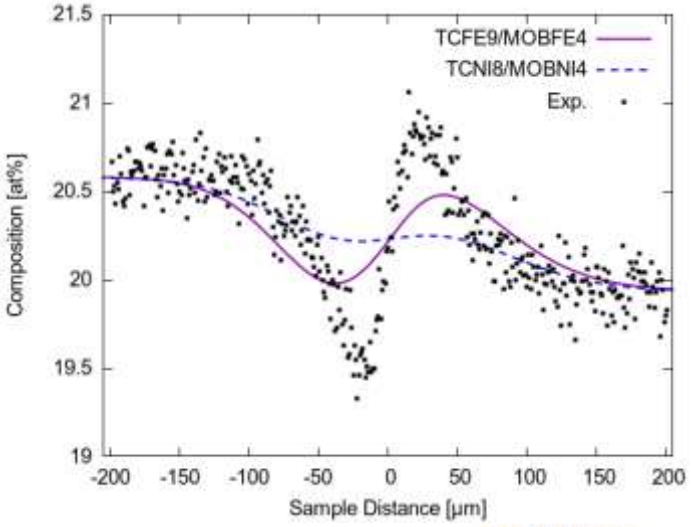
Cr



Fe



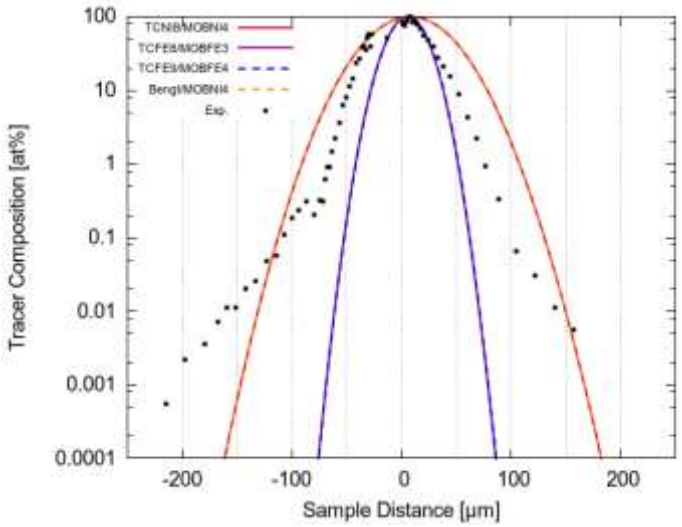
Mn



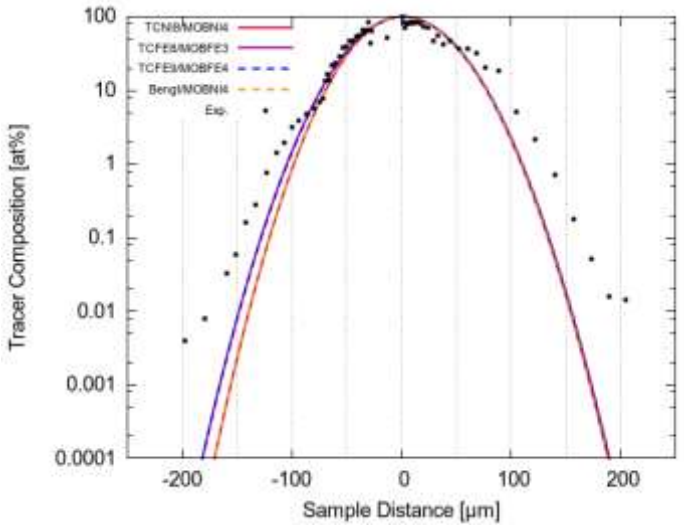
Example CoCrFeMnNi: Tracer Profiles

$Co_{25}CrFeMnNi_{15}$	$Co_{15}CrFeMnNi_{25}$

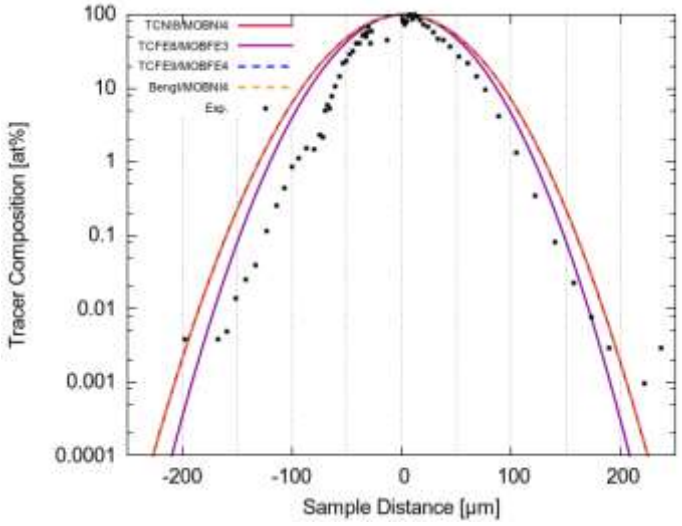
Co



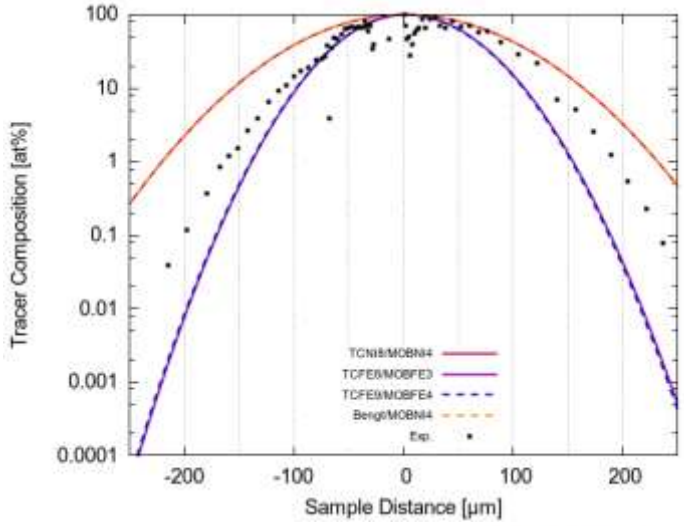
Cr



Fe



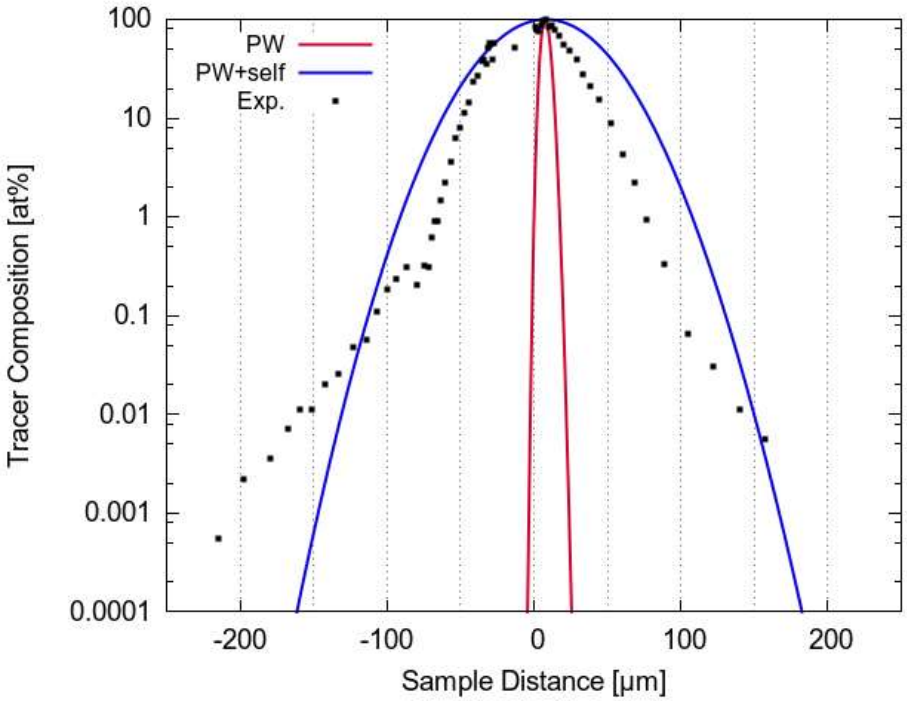
Mn



Example CoCrFeMnNi: Influence of Interdiffusion TCNI8/MOBNI4

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

Co: Influence of single diffusion models



Blue: Self-diffusion + interdiffusion

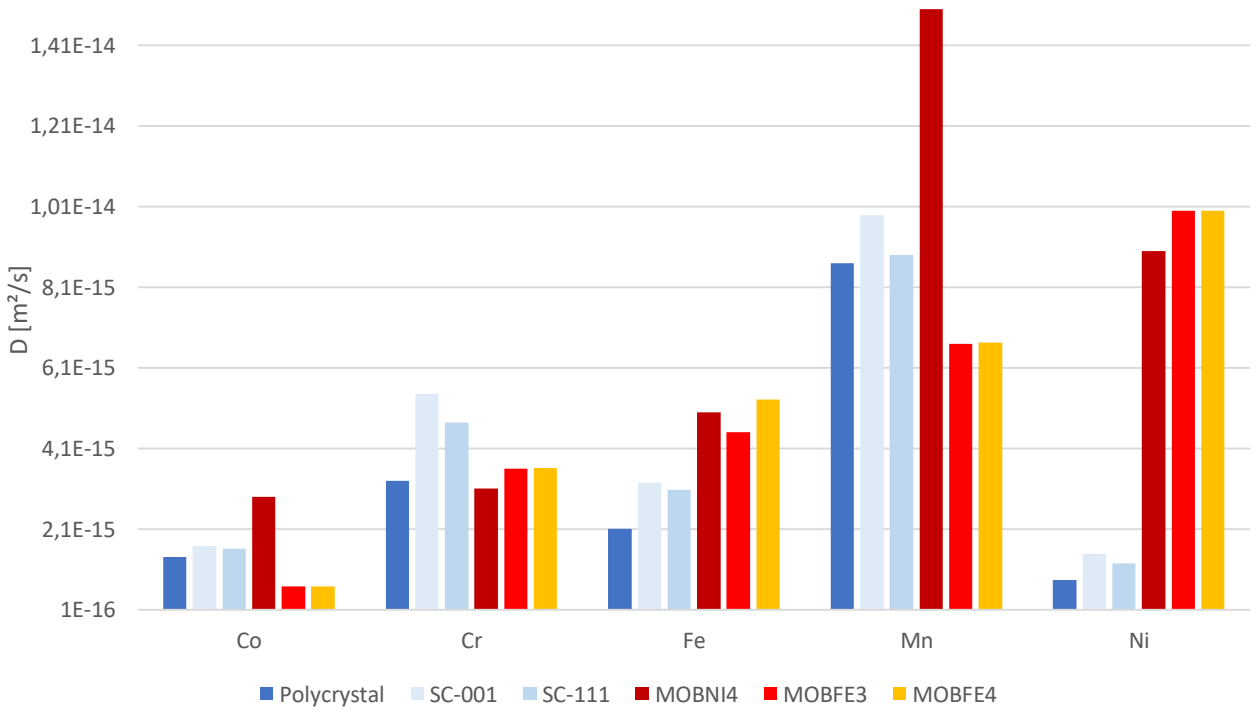
Red: No self-diffusion; only interdiffusion

→ Influence of interdiffusion on the tracer profile is small

→ Interdiffusion leads to a shift of the tracer profile

Comparison of self-diffusion coefficients

$Co_{20}Cr_{20}Fe_{20}Ni_{20}Mn_{20}$

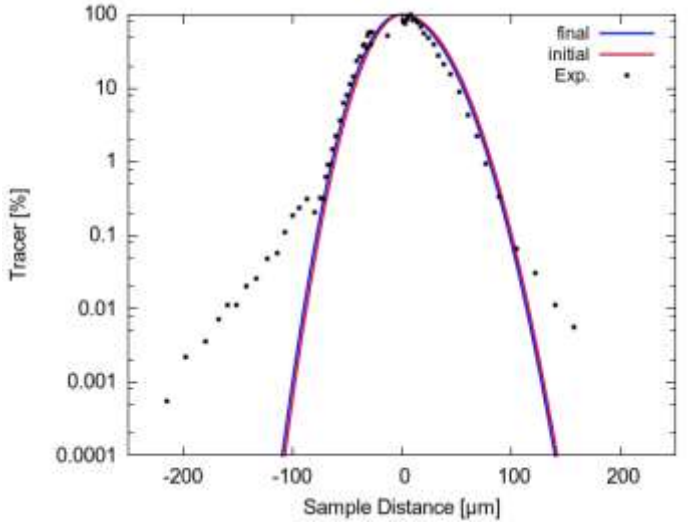


- Deviations of kinetic databases from experiments in concentrated alloys
  → use experimentally measured diffusion coefficients
- Effect of interdiffusion on the tracer profile is small
  → Skip interdiffusion and only use self-diffusion

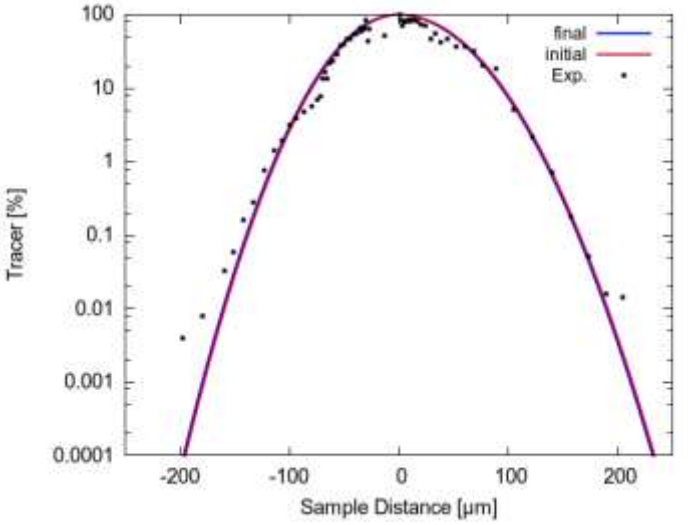
Example CoCrFeMnNi: Only self-diffusion, fixed overall concen

$Co_{25}CrFeMnNi_{15}$	$Co_{15}CrFeMnNi_{25}$

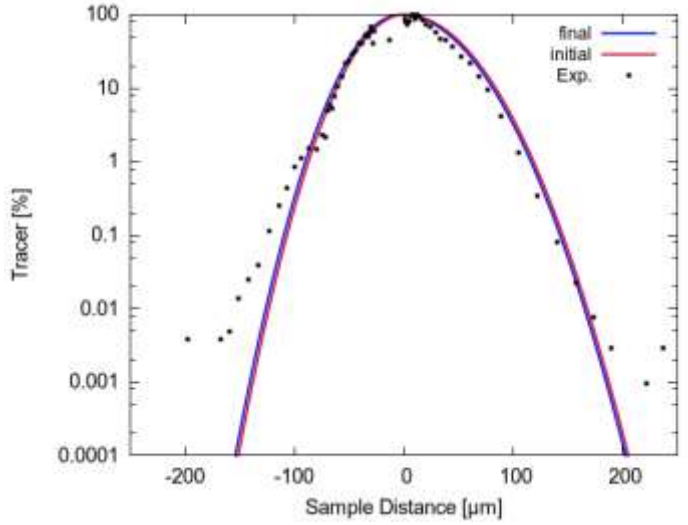
Co



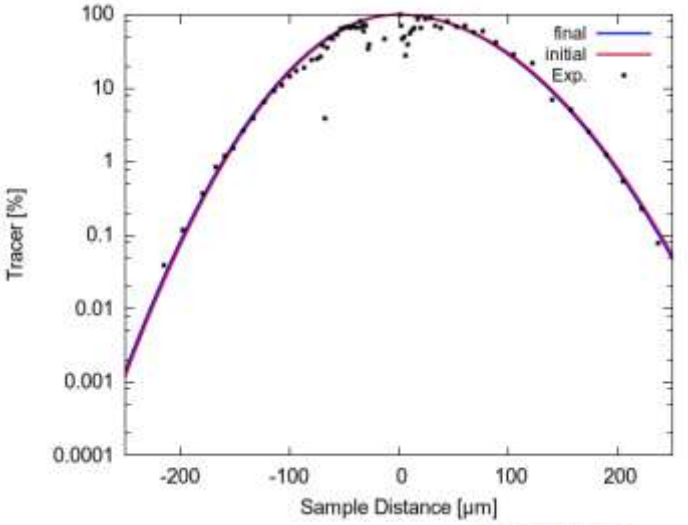
Cr



Fe

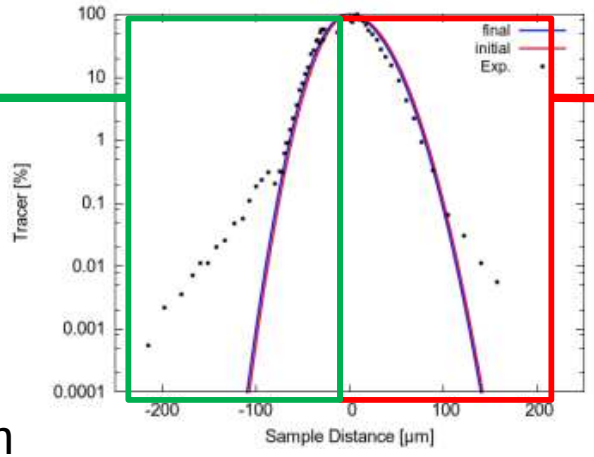


Mn

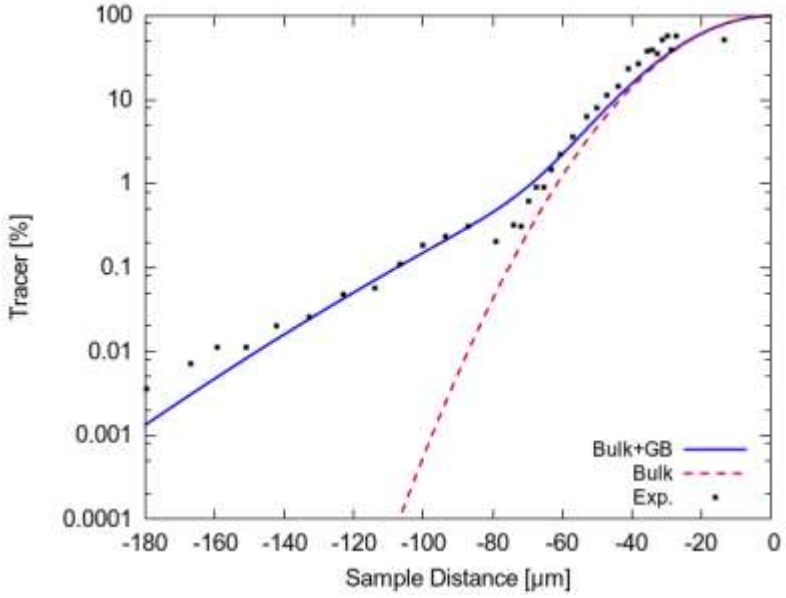


Example CoCrFeMnNi: Simulation results Co

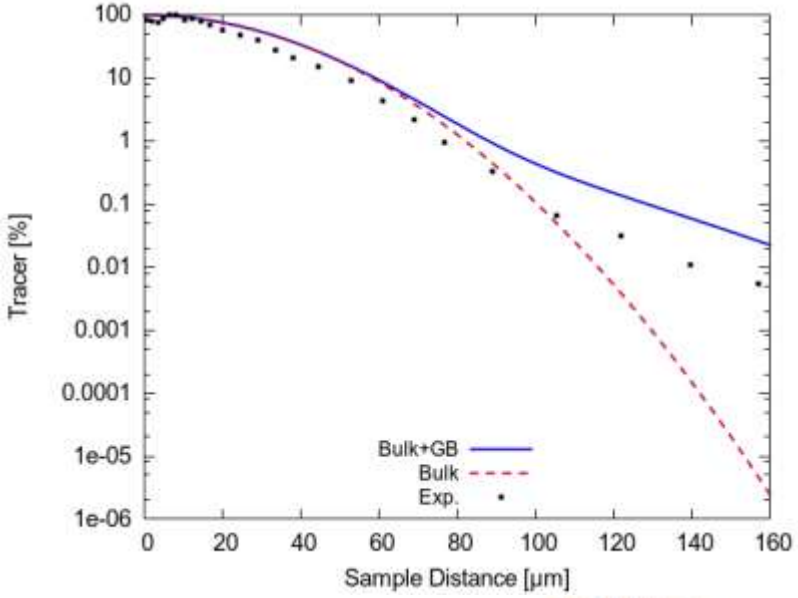
$Co_{25}CrFeMnNi_{15}$	$Co_{15}CrFeMnNi_{25}$



- Initial profile
- Grain size: 400 µm
- Increase on GB: 150000



- Initial profile
- Grain size: 600 µm
- Increase on GB: 150000



Summary and Outlook

- Diffusion models (not limited in number of components):
  - Interdiffusion
  - Self-diffusion
  - Faster diffusion on grain boundaries

→ Investigate their influence on measured profiles

- More theoretical:
  - Understand diffusion mechanism in concentrated multicomponent alloys

  → Diffusion model
  - Validate influence of kinetic cross terms

- Use theoretical knowledge:
  - Mobility database
  - Use diffusion experiments to check thermodynamic databases

- Use diffusion information for nucleation and growth of compound phases