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

• No combination with self-diffusion model
New simulation methods

**Interdiffusion**

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

- 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
Tracer atoms
Grain Boundary

Final
Grain Boundary

Graph showing the comparison between simulation and experiment over sample distance.
Example CoCrFeMnNi

$^{57}\text{Co}, ^{51}\text{Cr}, ^{59}\text{Fe}, ^{54}\text{Mn} \rightarrow \gamma$ - radiators

$\text{Co}_{25}\text{CrFeMnNi}_{15}$  $\text{Co}_{15}\text{CrFeMnNi}_{25}$

Annealing time: 48 h
Annealing temperature 1373 K
Polycrystalline material
Example CoCrFeMnNi: Interdiffusion

Co

Cr

Fe

Mn
Example CoCrFeMnNi: Tracer Profiles
Example CoCrFeMnNi: Influence of Interdiffusion TCNI8/MOBNi4

Co: Influence of single diffusion models

→ Influence of interdiffusion on the tracer profile is small
→ Interdiffusion leads to a shift of the tracer profile

Blue: Self-diffusion + interdiffusion
Red: No self-diffusion; only interdiffusion
Comparison of self-diffusion coefficients

- 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 concentrations

Co:

Cr:

Fe:

Mn:
Example CoCrFeMnNi: Simulation results Co

- 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