Modelling of High Entropy Alloys

D. Utt, A. Stukowski, K. Albe

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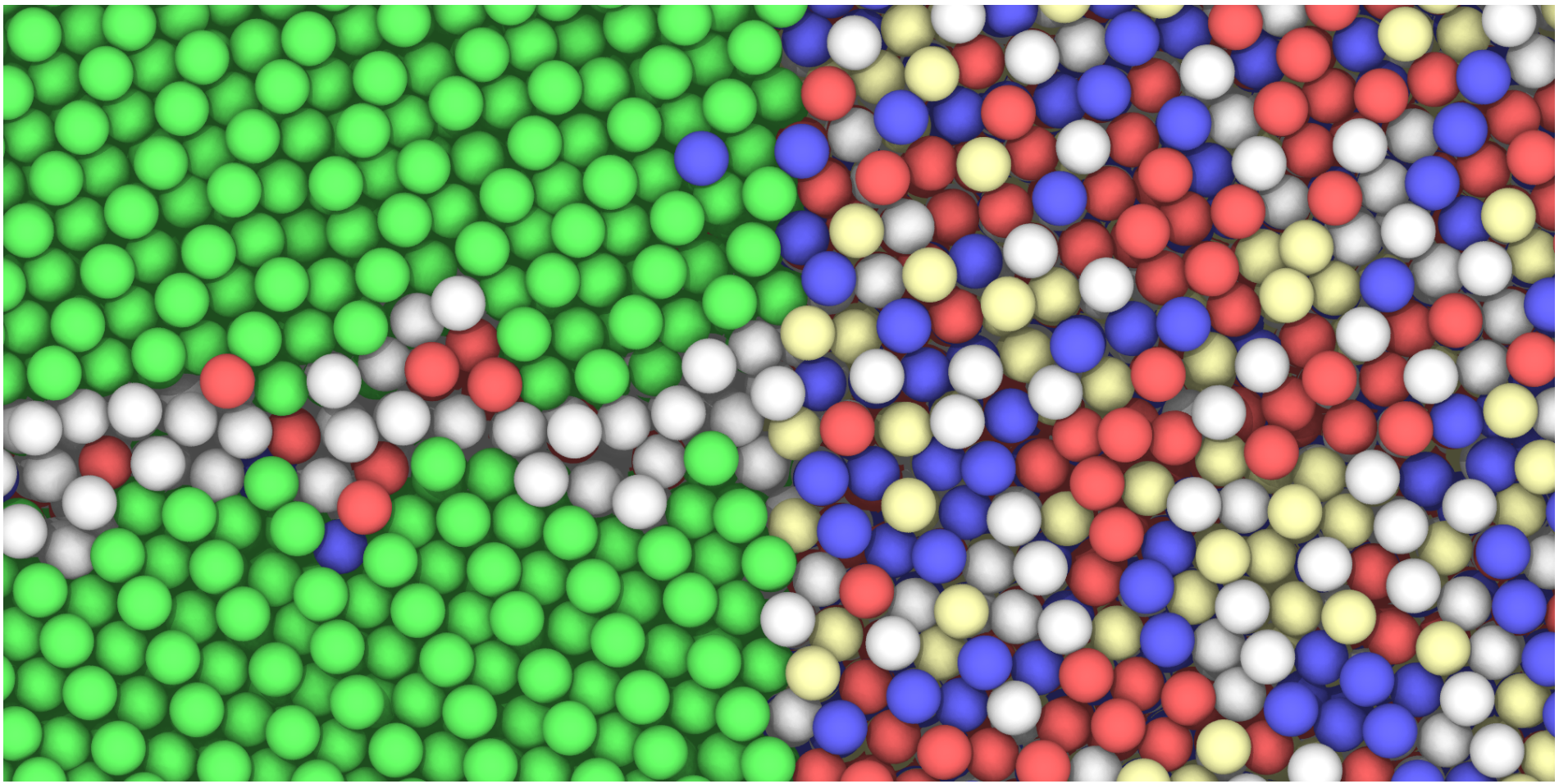

Overview

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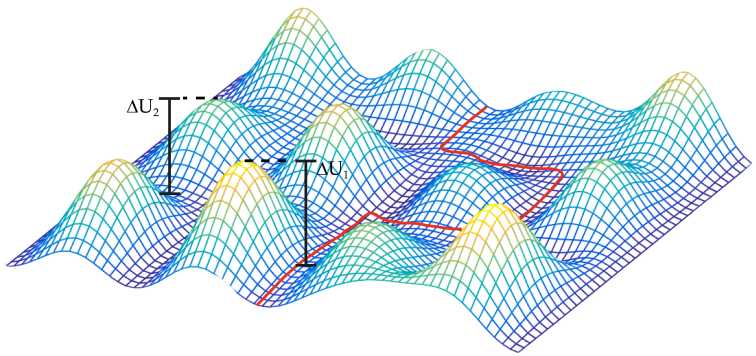
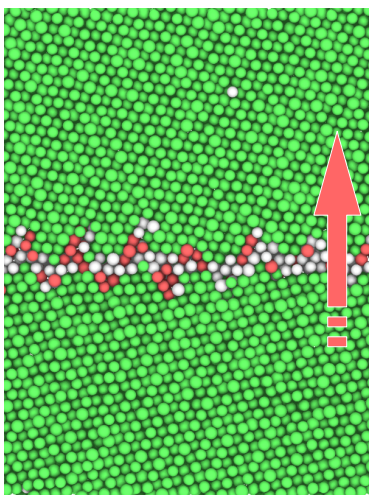
Understanding plasticity and microstructural evolution in FCC HEAs as near or mean field properties:

Solute strengthening as function of the composition.
Tom Keil at PhM, TU Darmstadt



Grain boundary migration under driven conditions.



Classical Theory of Solute Strengthening

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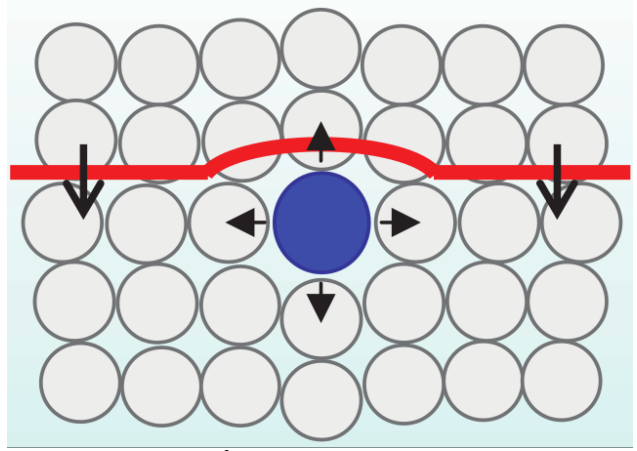
- Solutes dispersed in a matrix
- Solutes act as pinning sites for the dislocation
- $\sigma = 1.26\mu \left(\frac{w}{b}\right)^{\frac{1}{3}} c^{\frac{2}{3}} \left(\frac{\hat{K}}{2E}\right)^{\frac{4}{3}}$



Lu *et al.*, *Science*, 324 **5925**, 2009

Argon, *Oxford Materials*, 2008

Dislocations in HEAs

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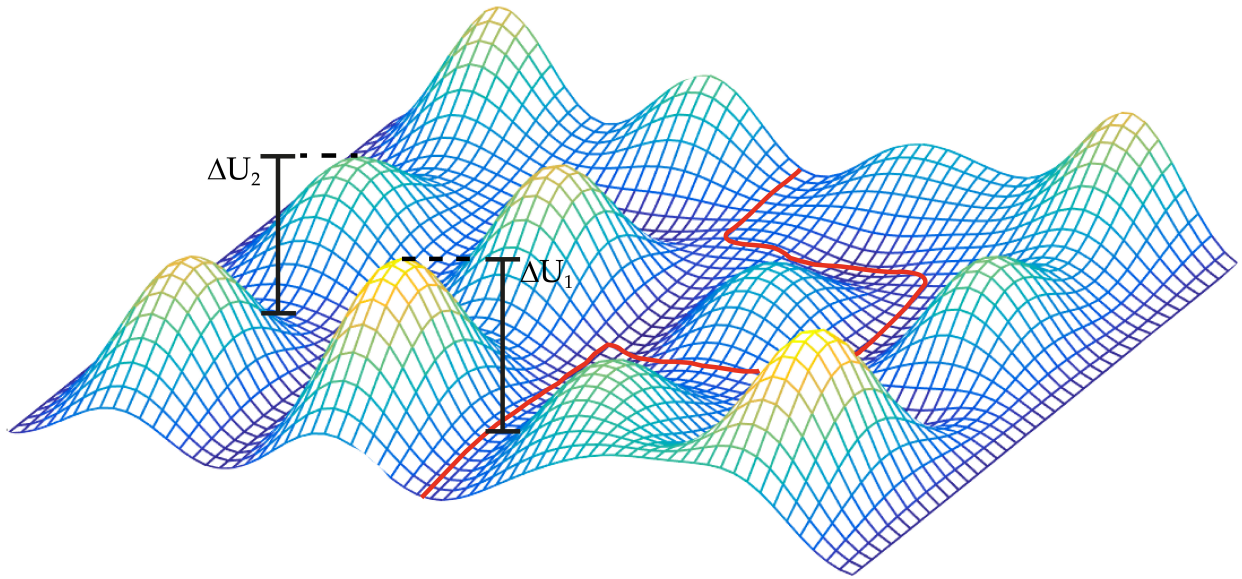
- Locally fluctuating energy landscape
- Dislocation line in a low energy configuration
- Pinning around the low energy points



Koch, *Master Thesis*, 2015

Dislocations in HEAs

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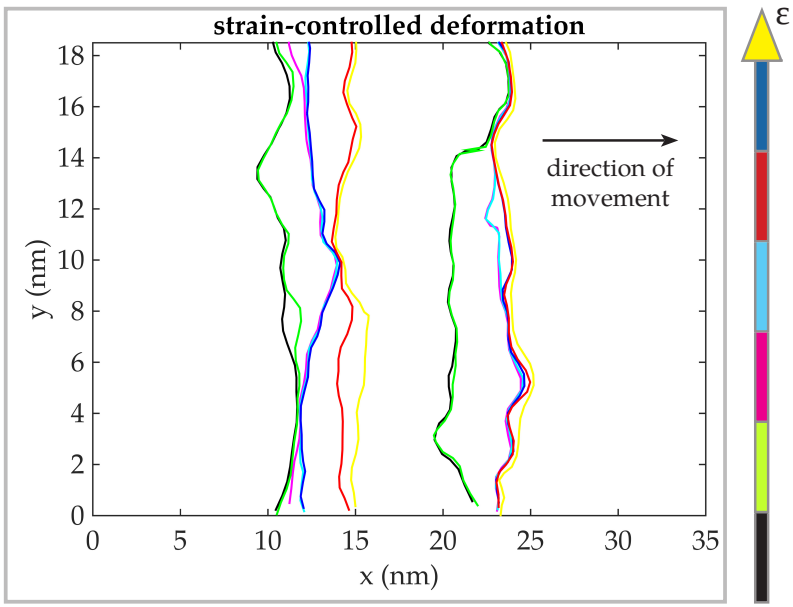
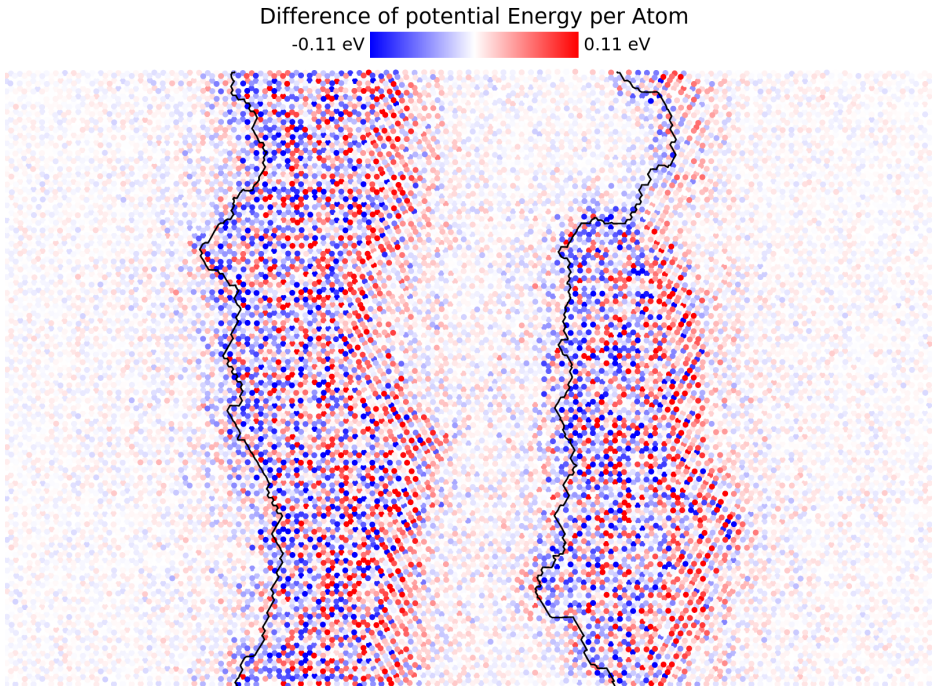
- Search for a local descriptor of dislocation pinning *e.g.* potential energy fluctuations.





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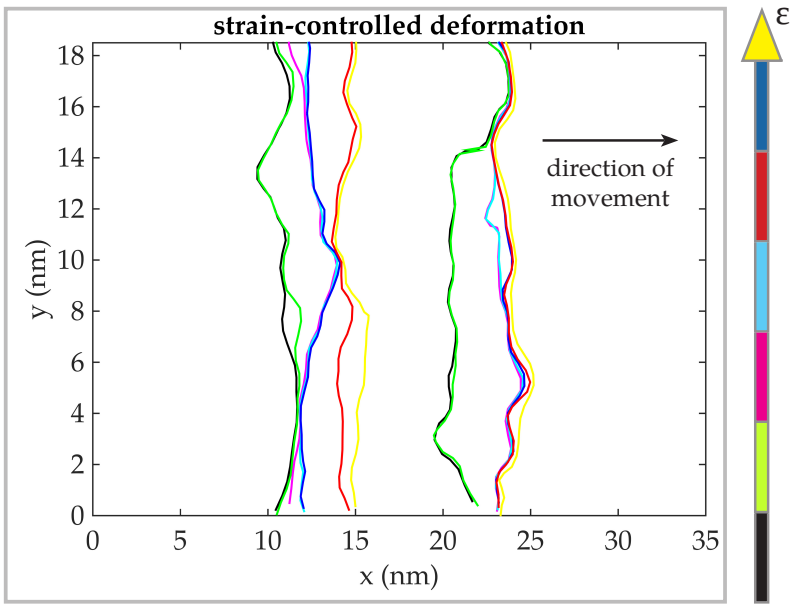

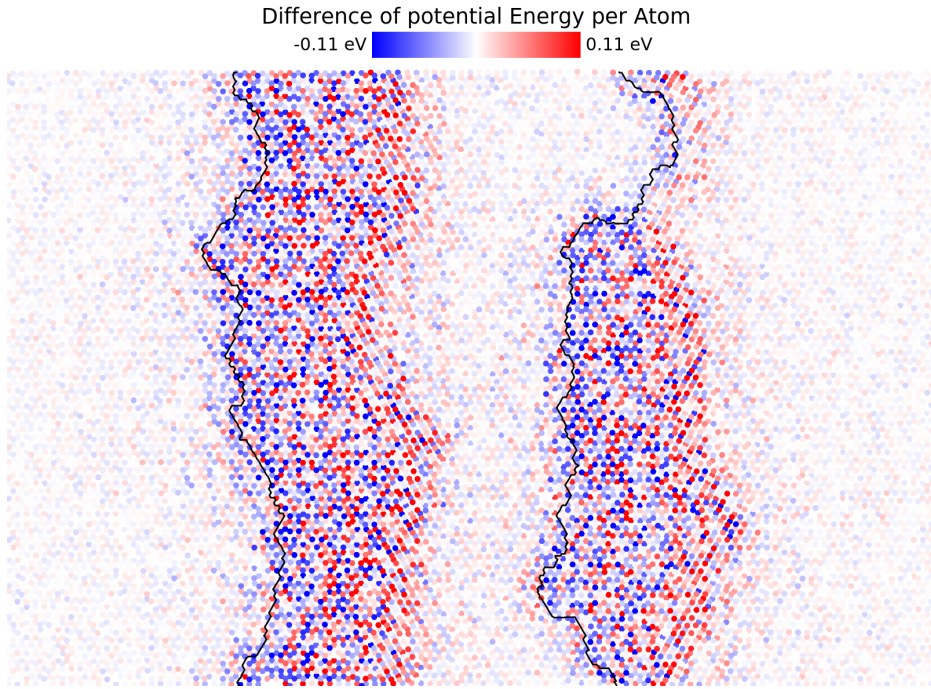

- We could not identify the nature of local pinning sites!

Koch, *Master Thesis*, 2015

Theory of Solute Strengthening in FCC HEAs

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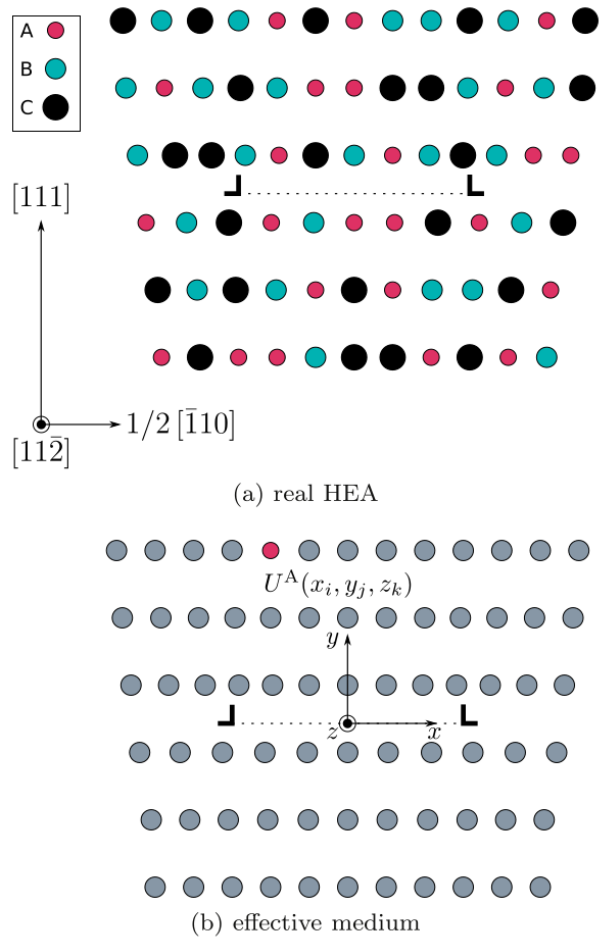
- Each alloy component is a solute in an average reference material
- Full model includes elastic and chemical interactions
- (Fitting) parameter-free



Varvenne *et al.*, *Acta Mater.*, 118, 2016

Theory of Solute Strengthening in FCC HEAs

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- The reduced model includes only elastic contributions
-

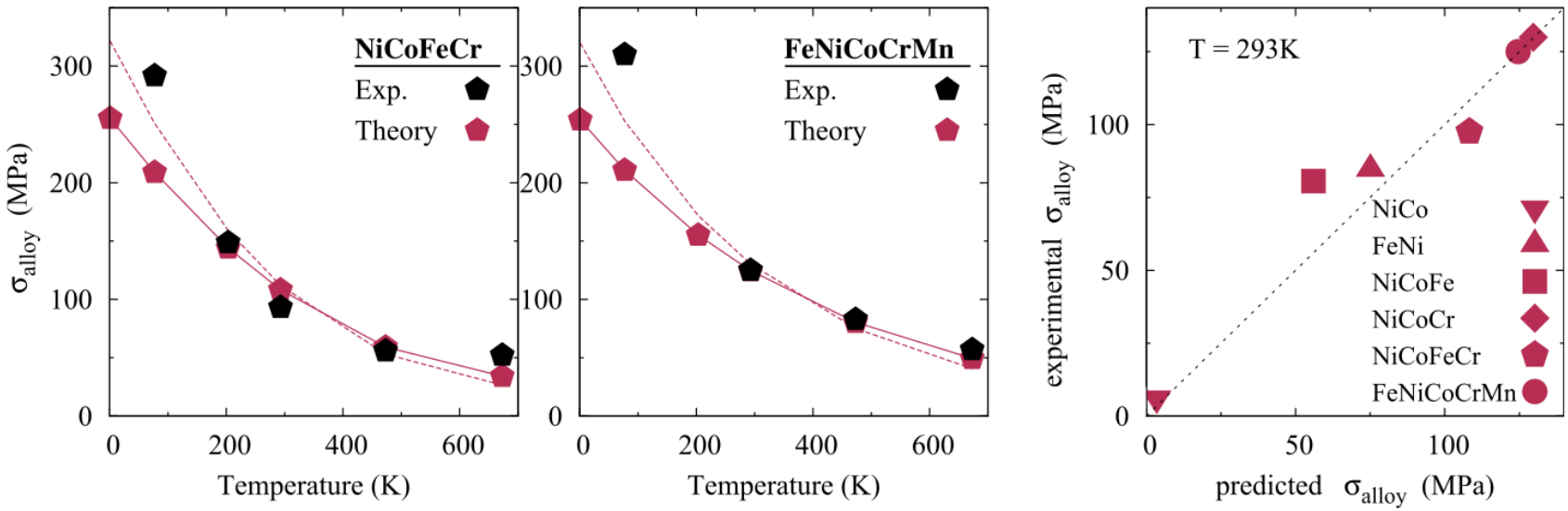
$$\tau_{y0} = 0.01785\alpha^{-1/3}\bar{\mu}\left(\frac{1+\bar{\nu}}{1-\bar{\nu}}\right)^{4/3}\left[\frac{\sum_n c_n \Delta V_n^2}{b^6}\right]^{2/3}$$

$$\Delta E_b = 1.5618\alpha^{1/3}\bar{\mu}b^3\left(\frac{1+\bar{\nu}}{1-\bar{\nu}}\right)^{2/3}\left[\frac{\sum_n c_n \Delta V_n^2}{b^6}\right]^{1/3}$$

$$\tau_y = \tau_{y0}\left[1-\left(\frac{k_B T}{\Delta E_b}\ln\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)^{1/3}\right]$$

Varvenne *et al.*, *Acta Mater.*, 118 2016

Theory of Solute Strengthening in FCC HEAs



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Solute Strengthening in FCC HEAs

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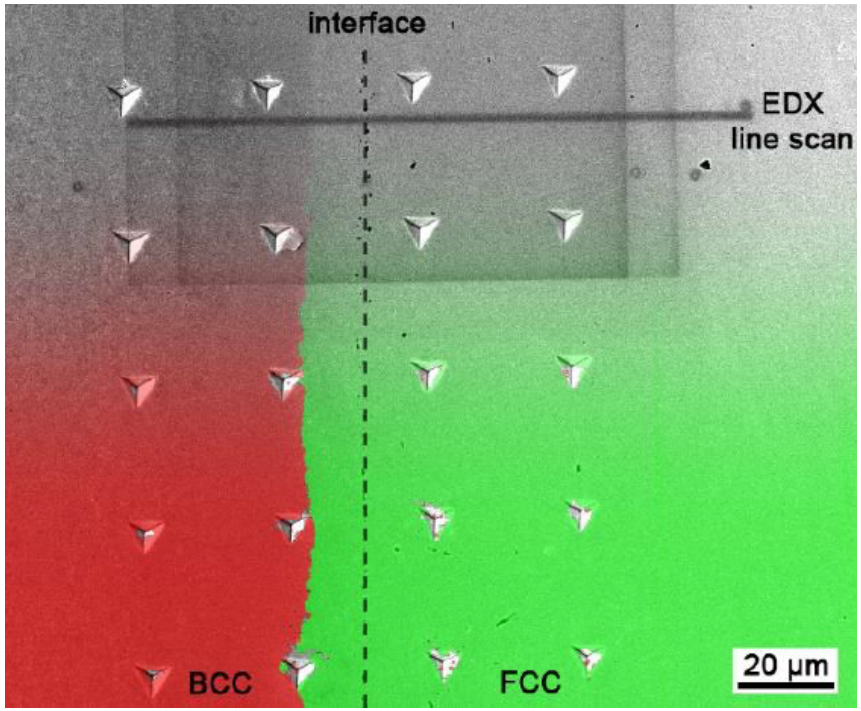
- Diffusion couples prepared and analyzed by Tom Keil, PhM TU Darmstadt

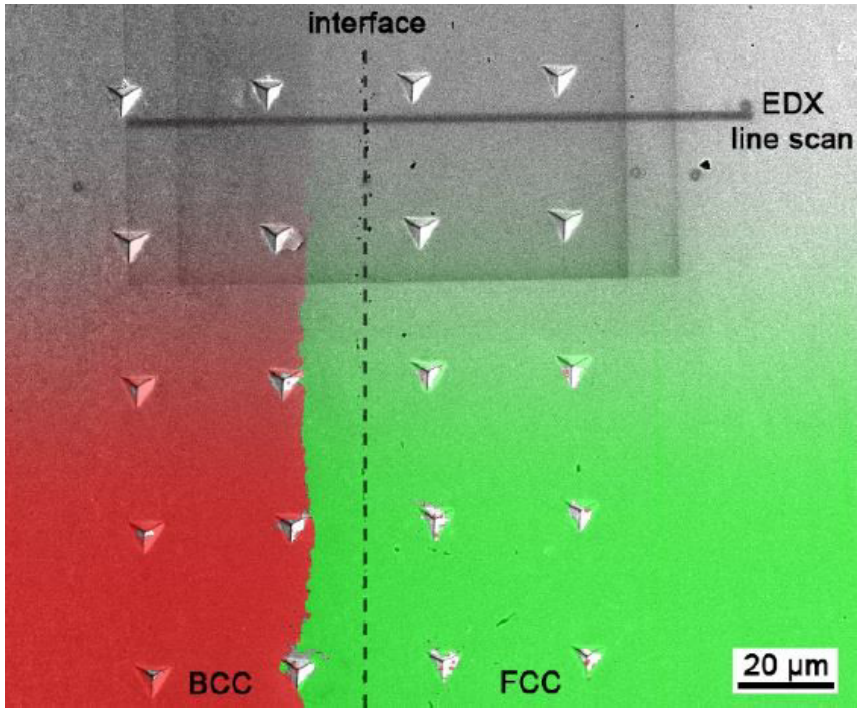


Poster: “Phase stability and solid solution strengthening of fcc high-entropy alloys”, Keil, Bruder, Durst

Solute Strengthening in FCC HEAs

TECHNISCHE UNIVERSITÄT DARMSTADT

- Diffusion couples prepared and analyzed by Tom Keil, PhM TU Darmstadt
- Solute strengthening in Cantor + Ni sample
- For detailed strength and phase stability determination of MP35N (CoNiCrMo) or Cantor alloy diffusion couples, visit his poster



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Strength in the Cantor + Ni Couple

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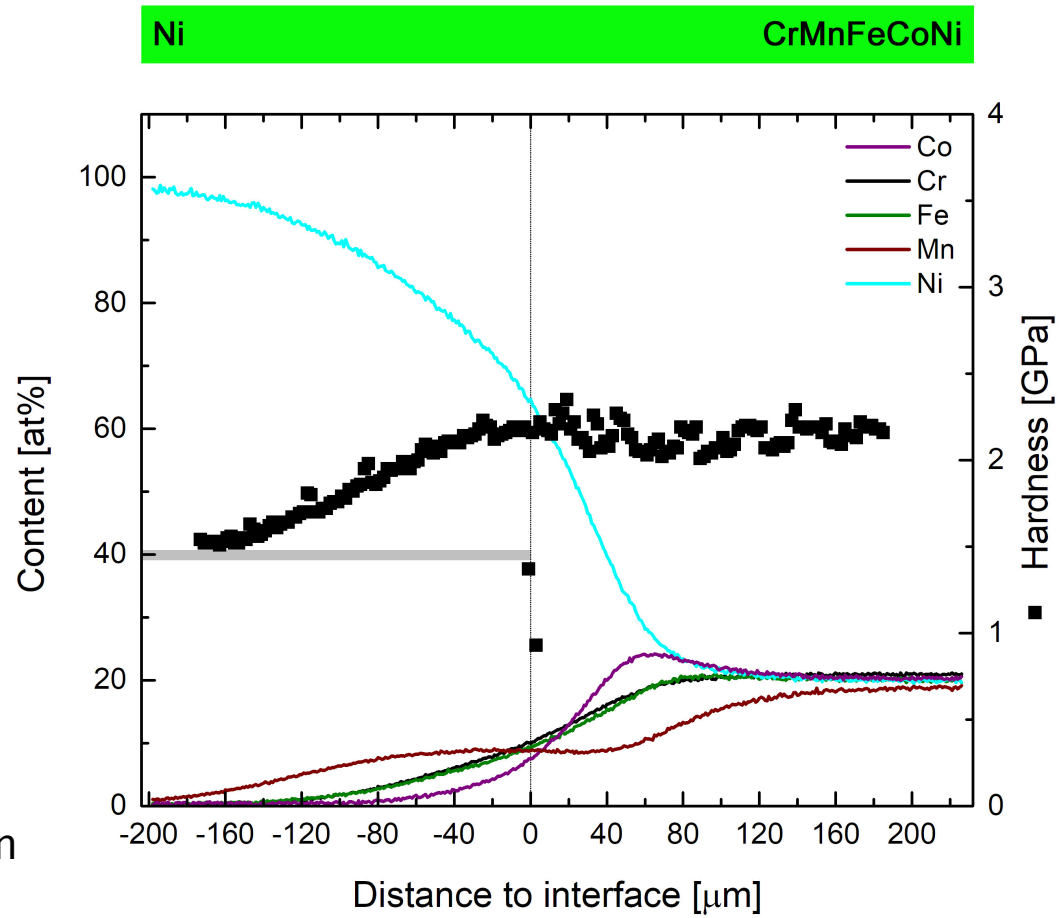
- Full FCC miscibility
- Hardness plateau in the Cantor alloy



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Strength in the Cantor + Ni Couple

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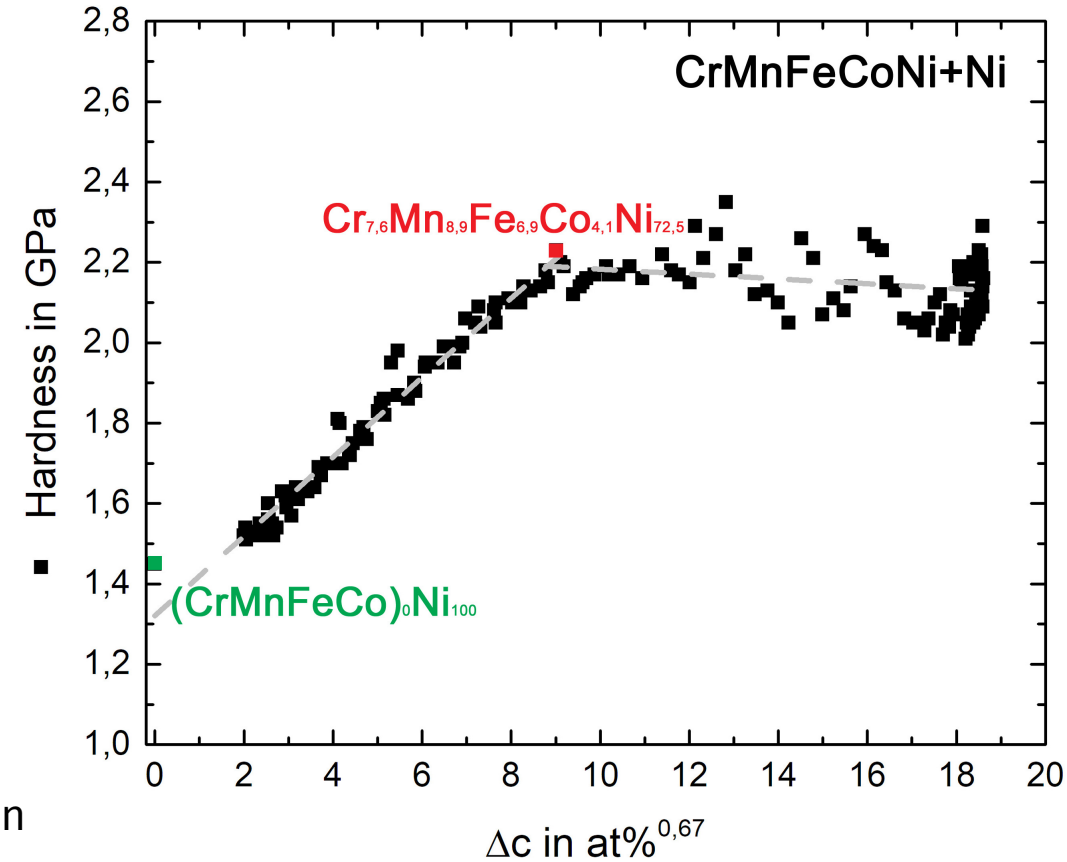
- Quasi-binary approach of the conventional solute strengthening model ($\sigma \propto c^{2/3}$)
- Two different fits required



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Strength in the Cantor + Ni Couple

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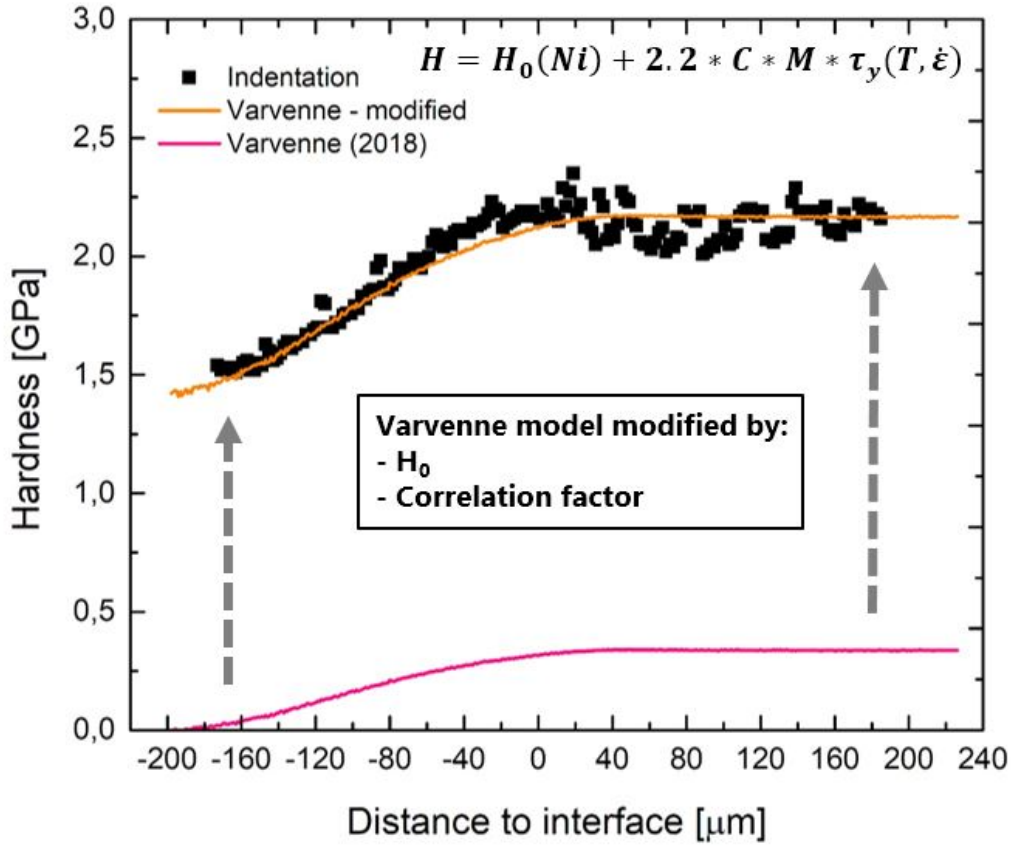
- All average matrix properties derived from rules of mixture



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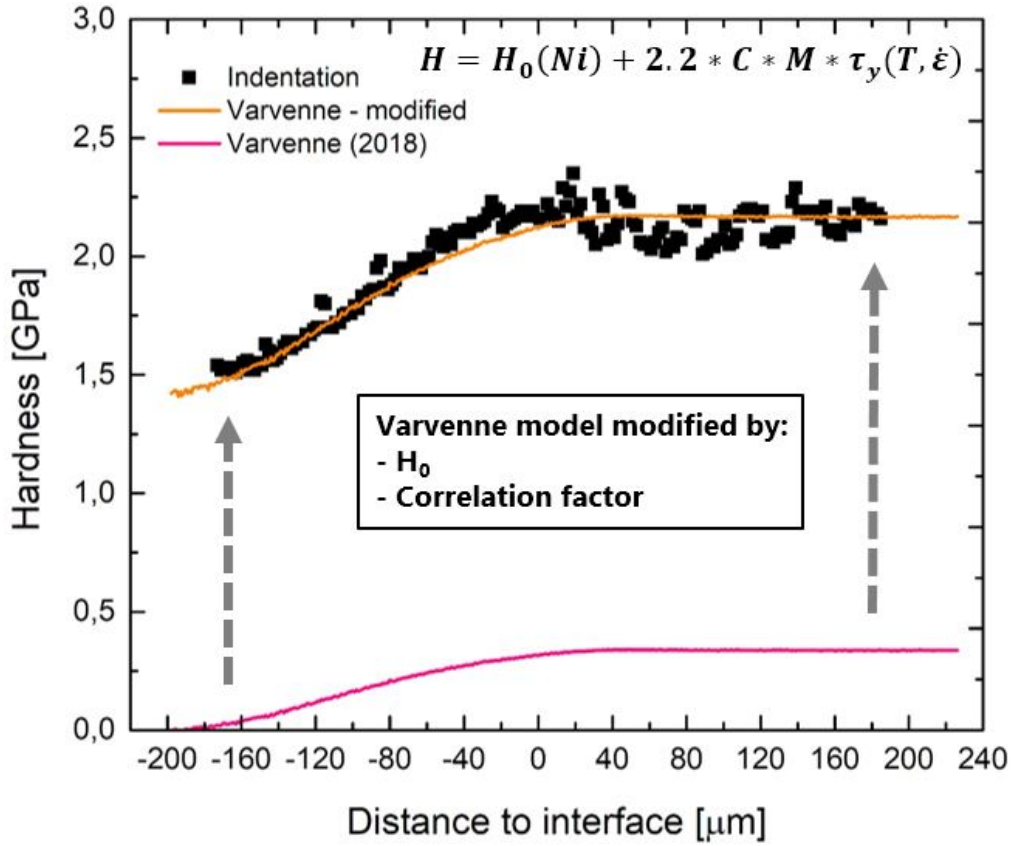
Strength in the Cantor + Ni Couple

TECHNISCHE UNIVERSITÄT DARMSTADT

- All average matrix properties derived from rules of mixture
- The solutes in average matrix approach describes the strength profile well.



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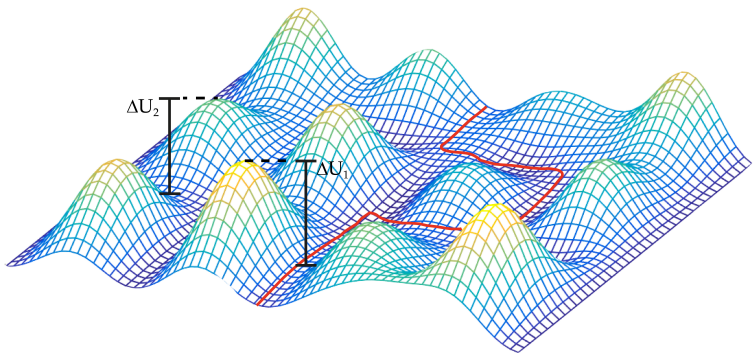

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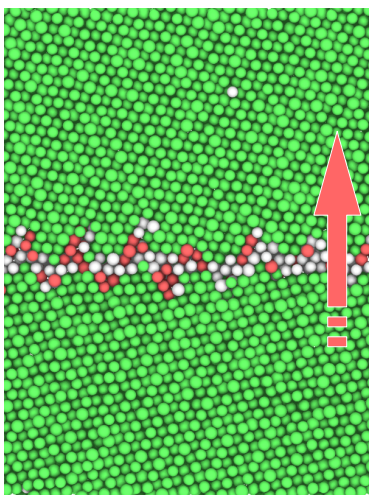


Methodology

TECHNISCHE UNIVERSITÄT DARMSTADT

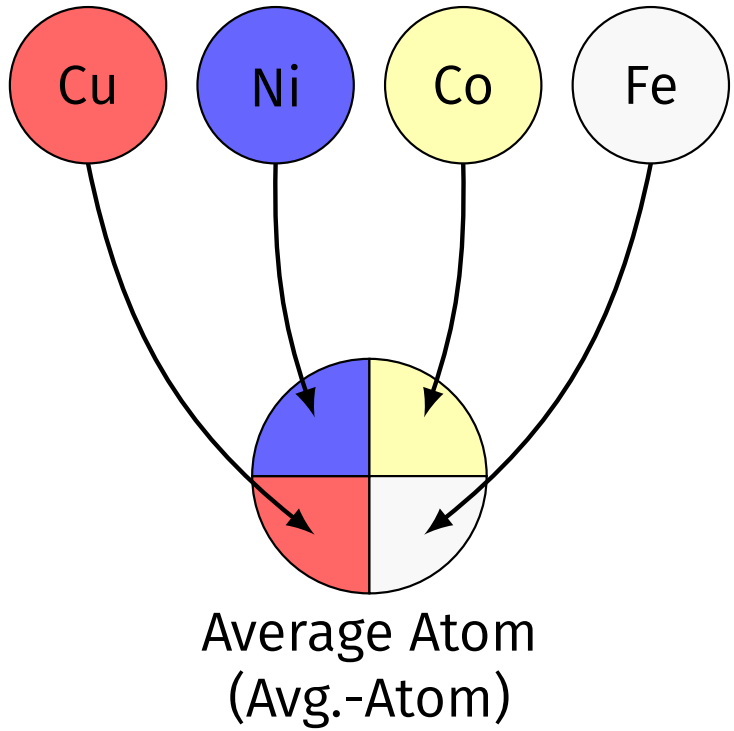
- Σ11 (332) <110> symmetrical tilt grain boundary
- FCC CuNiCoFe model HEA
- Atomistic simulations using LAMMPS

Zhou *et al.*, *Phys. Rev. B*, 2004, 69; Varvenne *et al.*, *Phys. Rev. B*, 2016, 93

Methodology

TECHNISCHE UNIVERSITÄT DARMSTADT

- Σ11 (332) <110> symmetrical tilt grain boundary
- FCC CuNiCoFe model HEA
- Atomistic simulations using LAMMPS
- Comparison to different pure metals and 'average atom'



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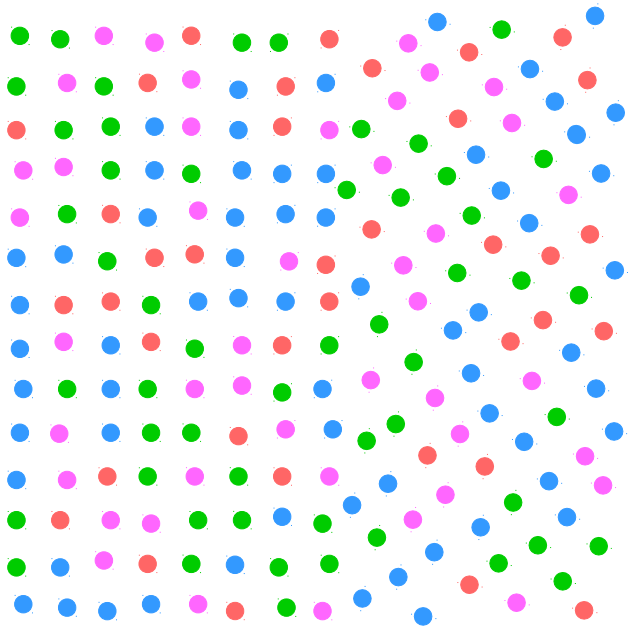
- Is the GB structure in the HEA modified by the lattice distortions?



Lattice Distortions

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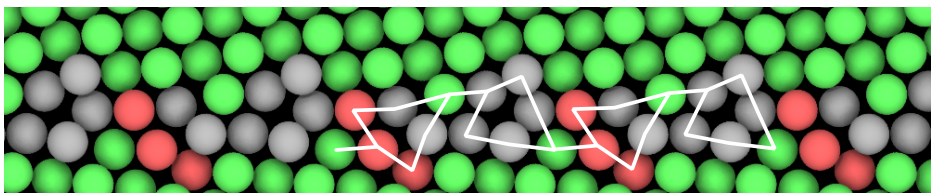
- Is the GB structure in the HEA modified by the lattice distortions?
- T = 0 K

•Other •FCC •HCP

Pure Cu



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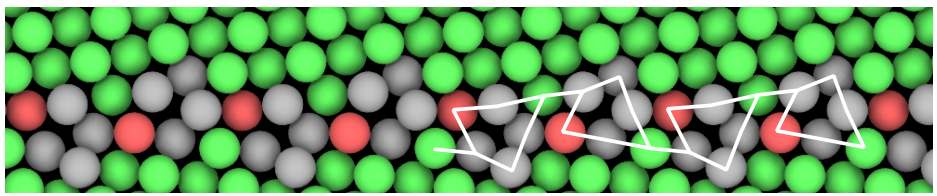
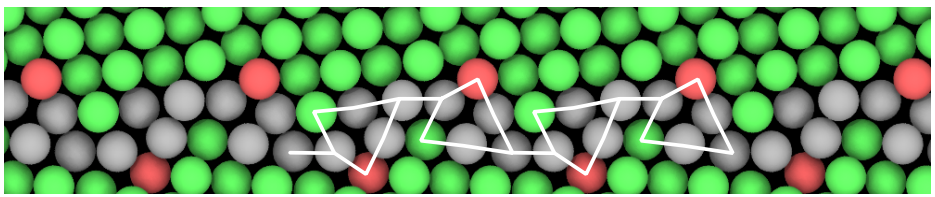


Pure average atom



Lattice Distortions

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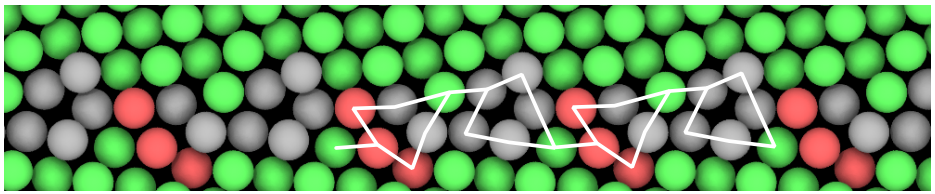

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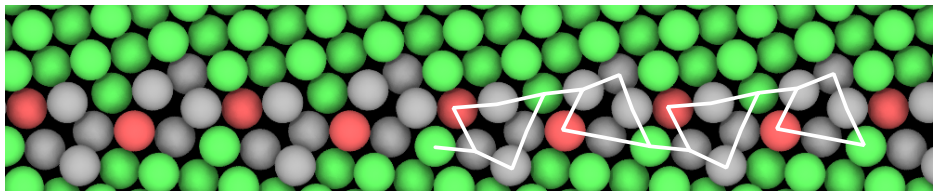

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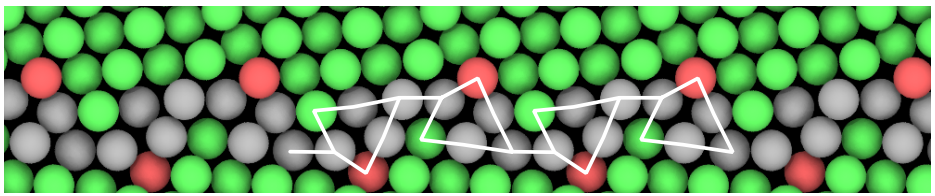
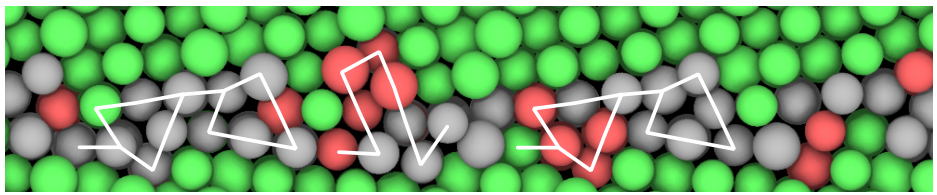


CuNiCoFe



Lattice Distortions

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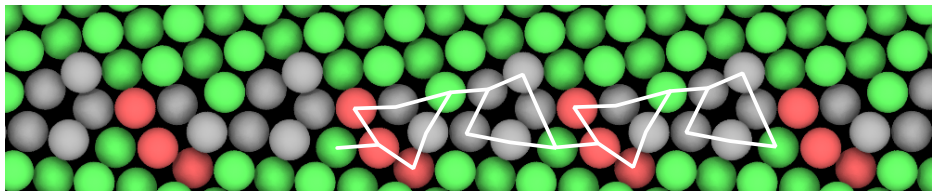

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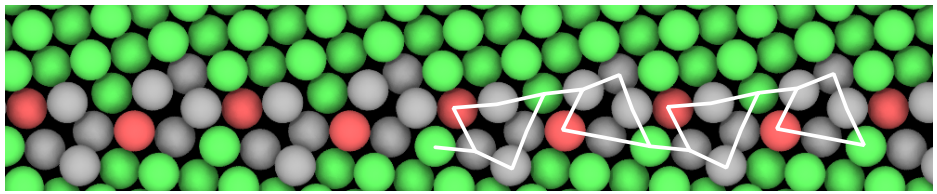

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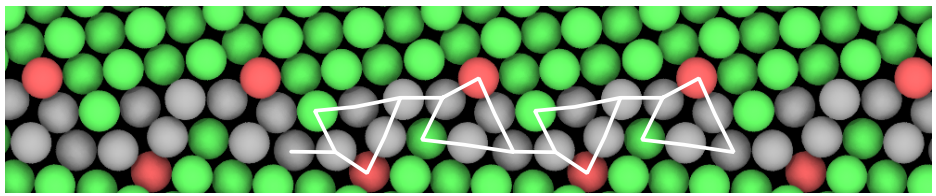

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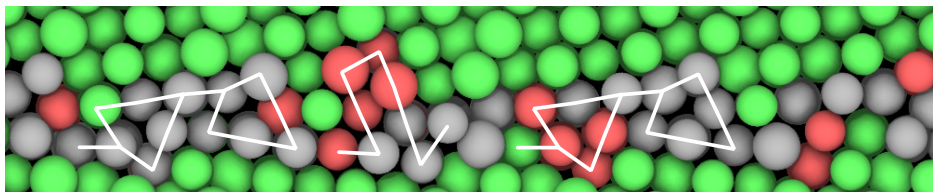

- There are only slight deviations from the ideal repeating units in the HEA at 0 K!

Lattice Distortions

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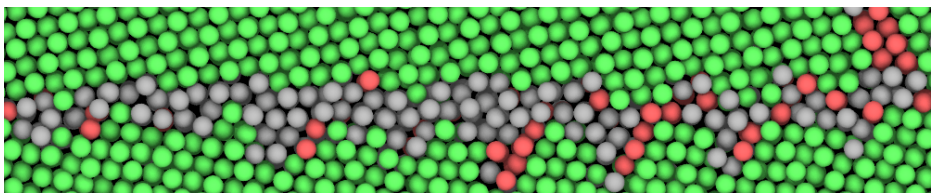
- Is the GB structure in the HEA modified by the lattice distortions?
- $T = 0.6 T_{melt}$

•Other •FCC •HCP

Pure Cu



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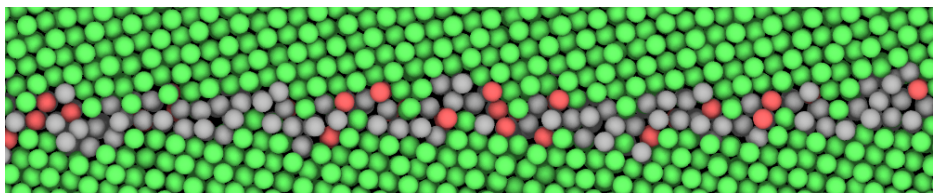

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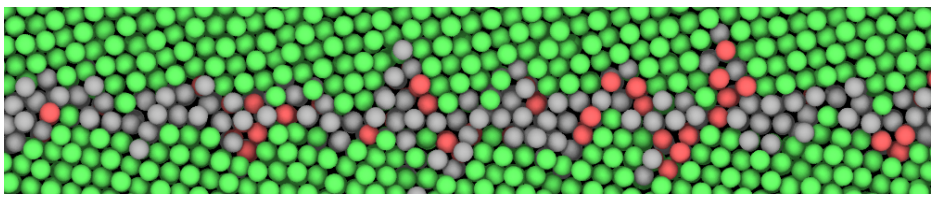

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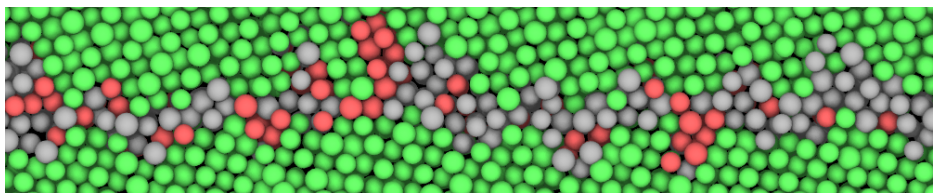

Lattice Distortions

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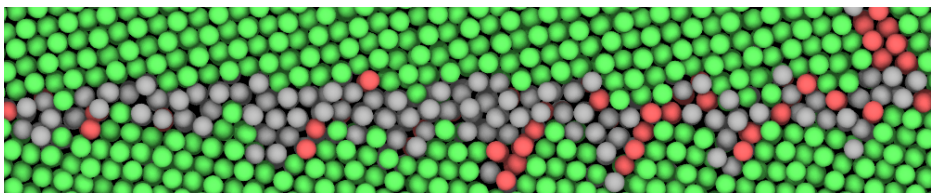

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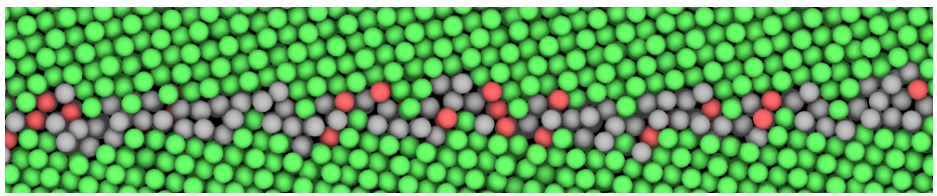

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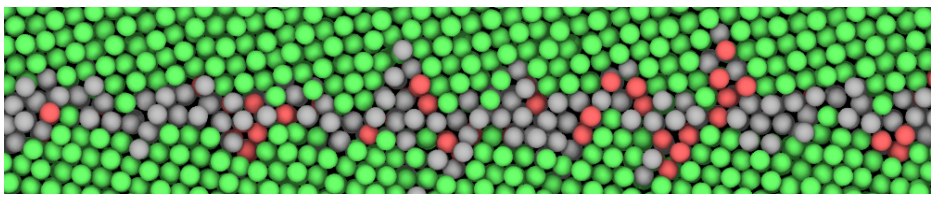

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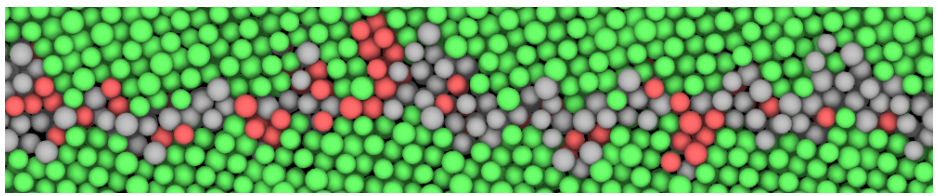
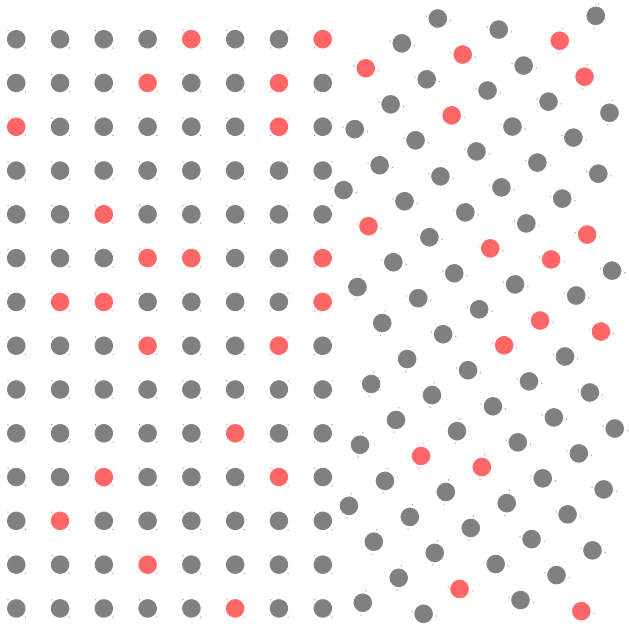


- The grain boundary structure at higher temperatures appears to be dominated by γ_{ISF} and γ_{USF}!

- Is the GB mobility in the HEA reduced by the local chemical fluctuations?



Methodology

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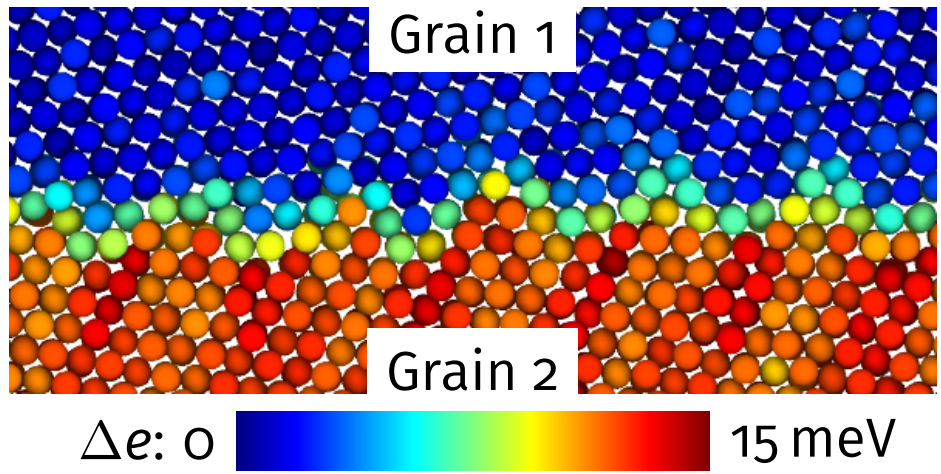

Janssens *et al.*, *Nat. Mater.*, 5 2006

Methodology

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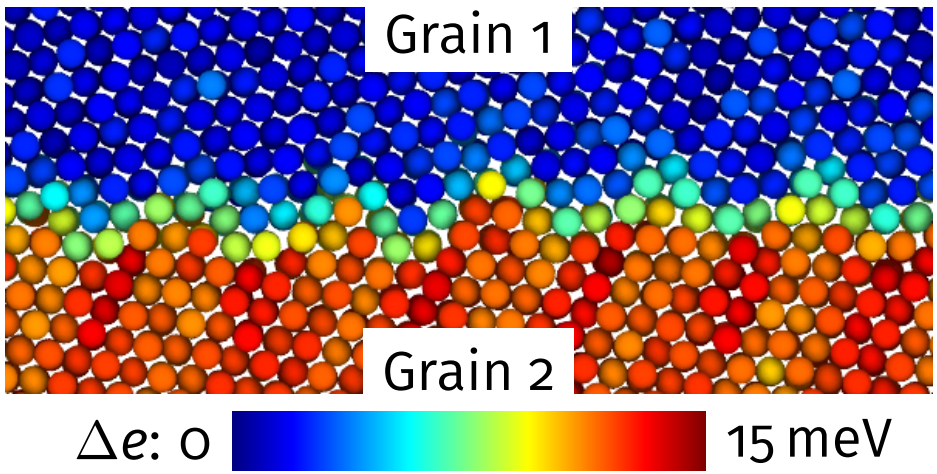
Synthetic driving pressure:

$$P = \frac{\Delta e}{\Omega}$$

GB Mobility:

$$M = \frac{v}{P}$$

$$M(T) = M^{\infty} \exp\left(\frac{-Q_m}{k_B T}\right)$$



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Σ11 STGB Mobility

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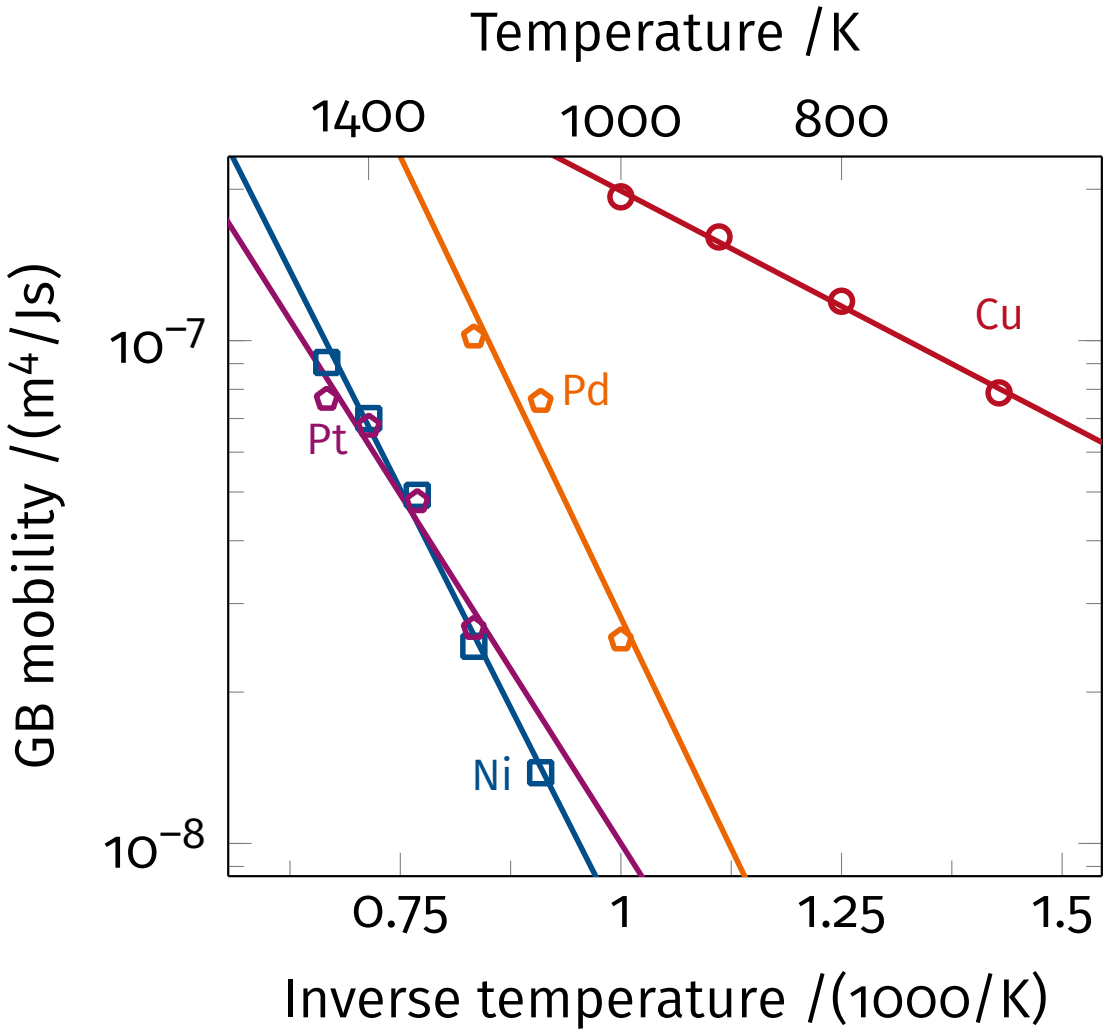

Σ11 STGB Mobility

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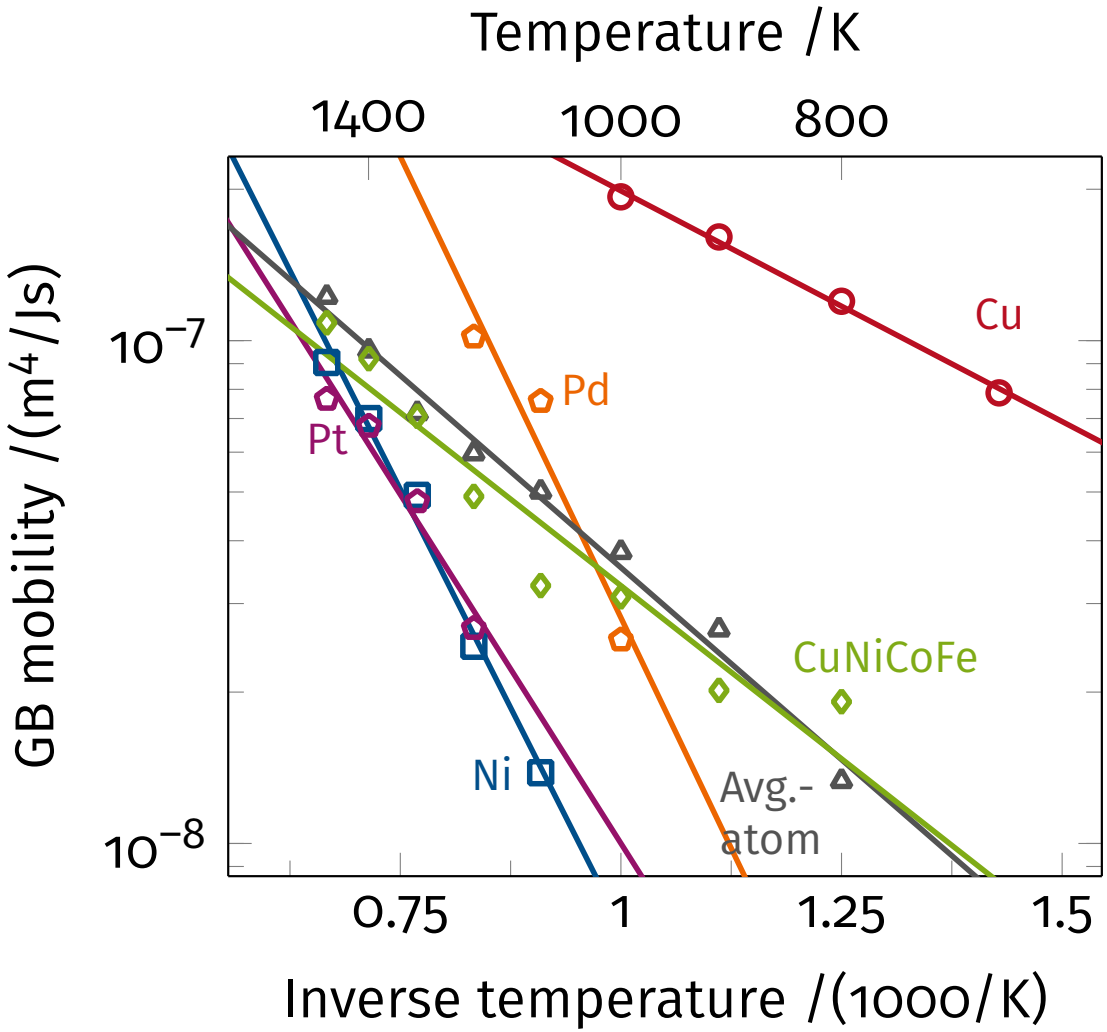
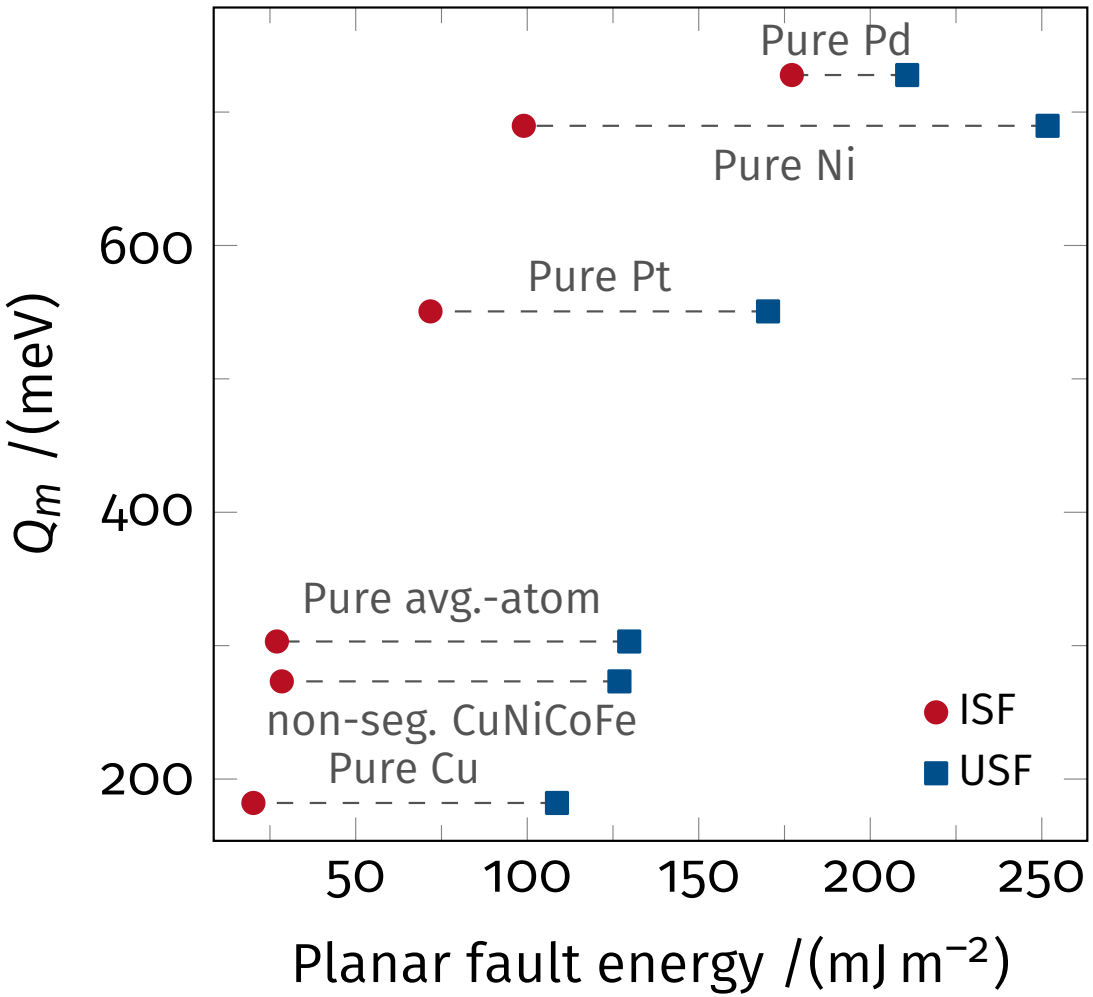
- Average atom and CuNiCoFe sample show almost identical mobilities



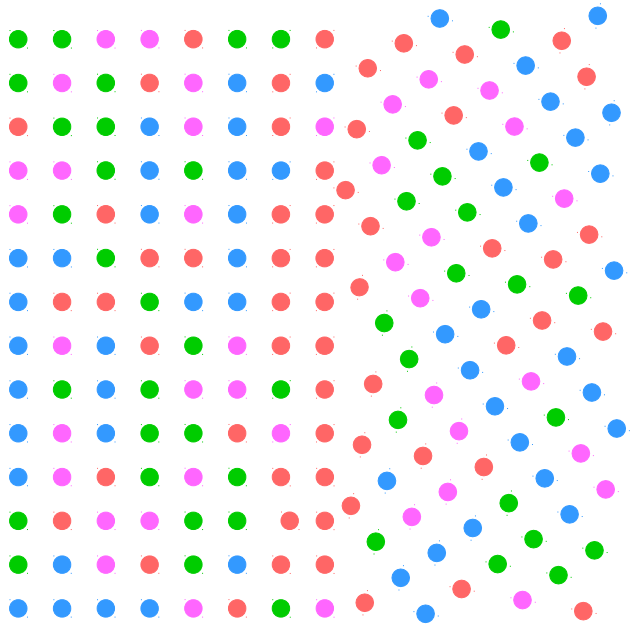
Σ11 STGB Mobility

TECHNISCHE UNIVERSITÄT DARMSTADT

- Average atom and CuNiCoFe sample show almost identical mobilities
- Activation barrier correlates strongly with γ_{ISF} and γ_{USF}!
- STGB migration via partial dislocations



- How does GB segregation impact the GB mobility?



Grain Boundary Segregation in the HEA

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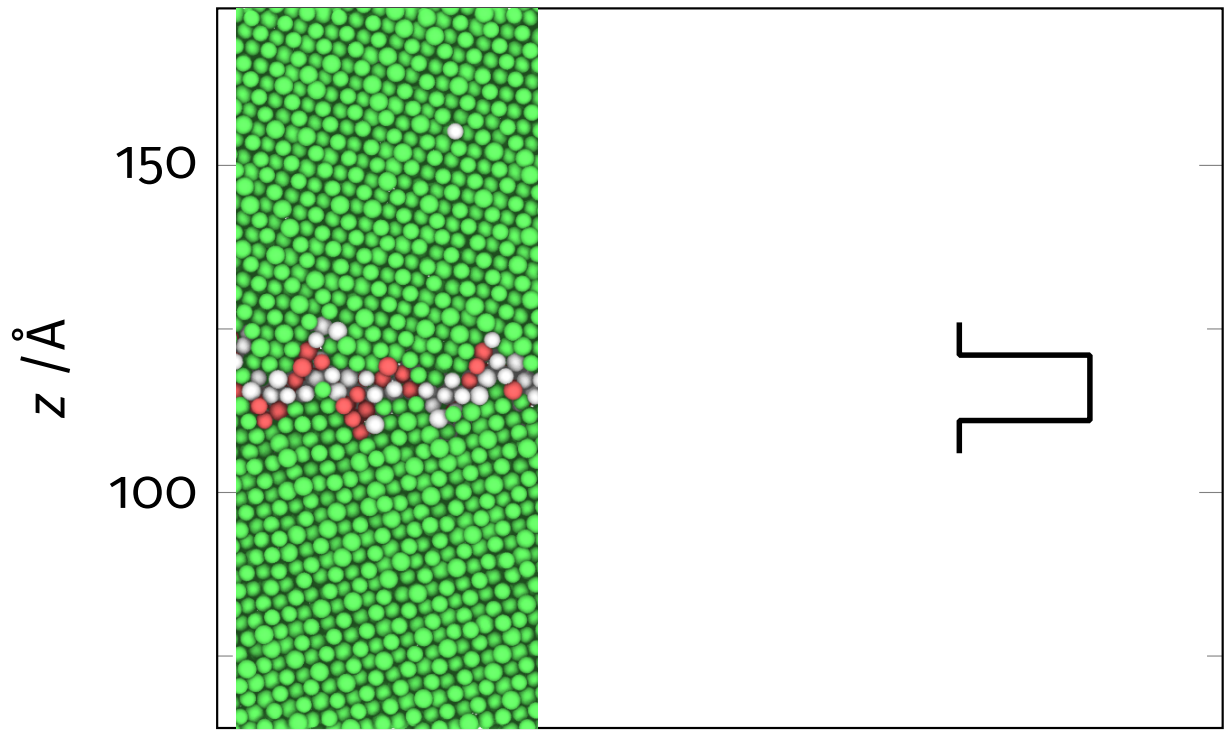
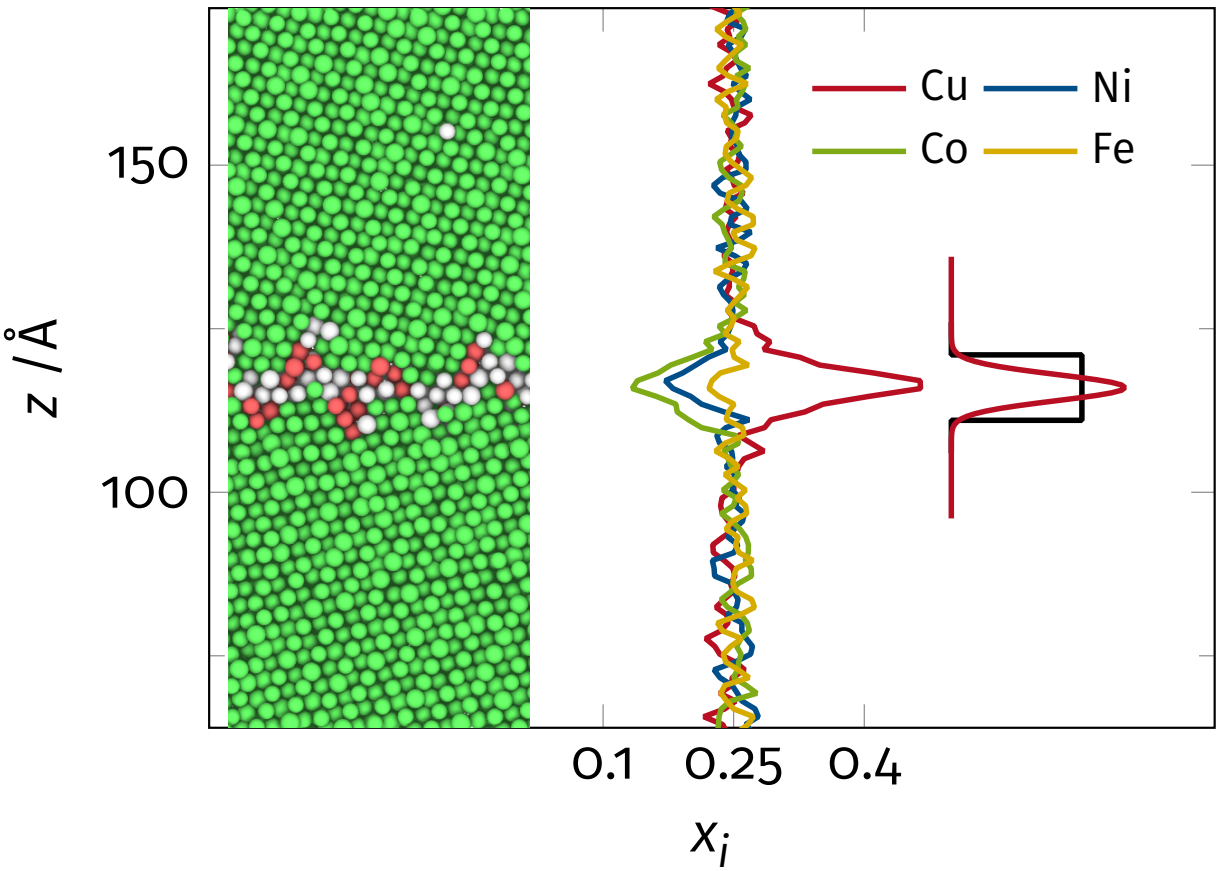
- $\Sigma 11$ STGB



Grain Boundary Segregation in the HEA

TECHNISCHE UNIVERSITÄT DARMSTADT

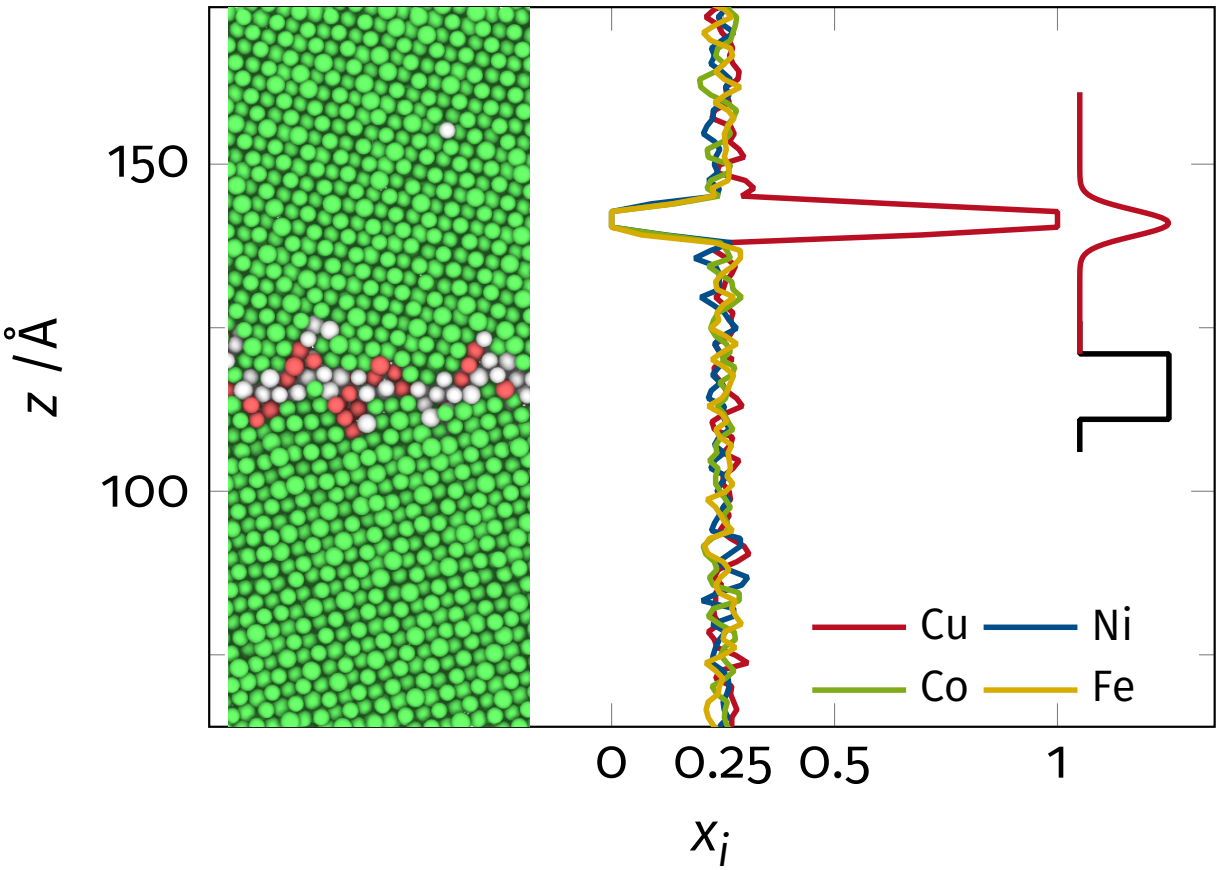
- $\Sigma 11$ STGB
- Monte-Carlo algorithm
- Seg. CuNiCoFe sample



Grain Boundary Segregation in the HEA

TECHNISCHE UNIVERSITÄT DARMSTADT

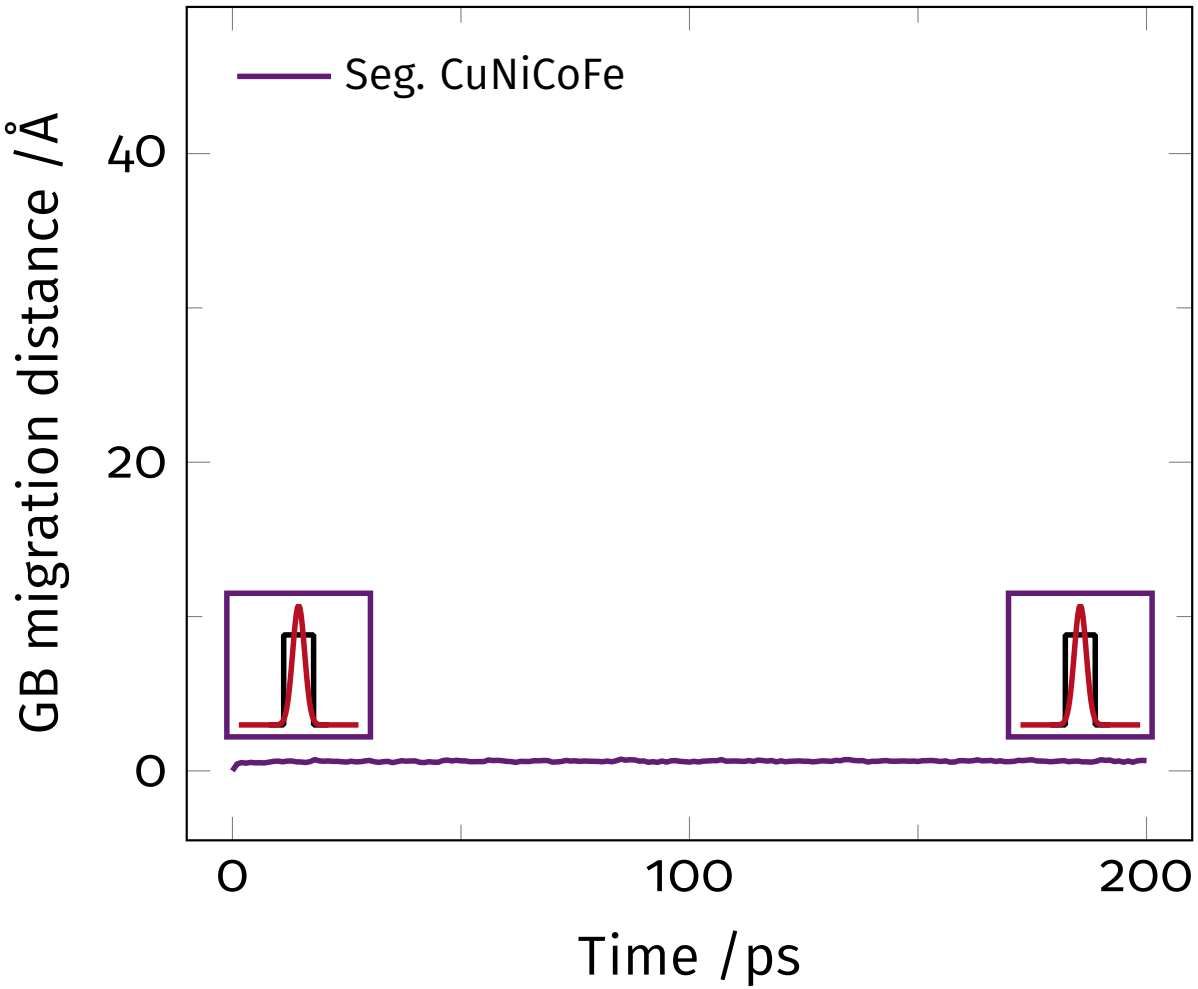
- $\Sigma 11$ STGB
- Monte-Carlo algorithm
- Seg. CuNiCoFe sample
- Artificially inserted Cu layer
- Art.-seg. CuNiCoFe sample



Grain Boundary Segregation in the HEA

TECHNISCHE UNIVERSITÄT DARMSTADT

- T = 1200 K
- Δe = 15 meV/atom



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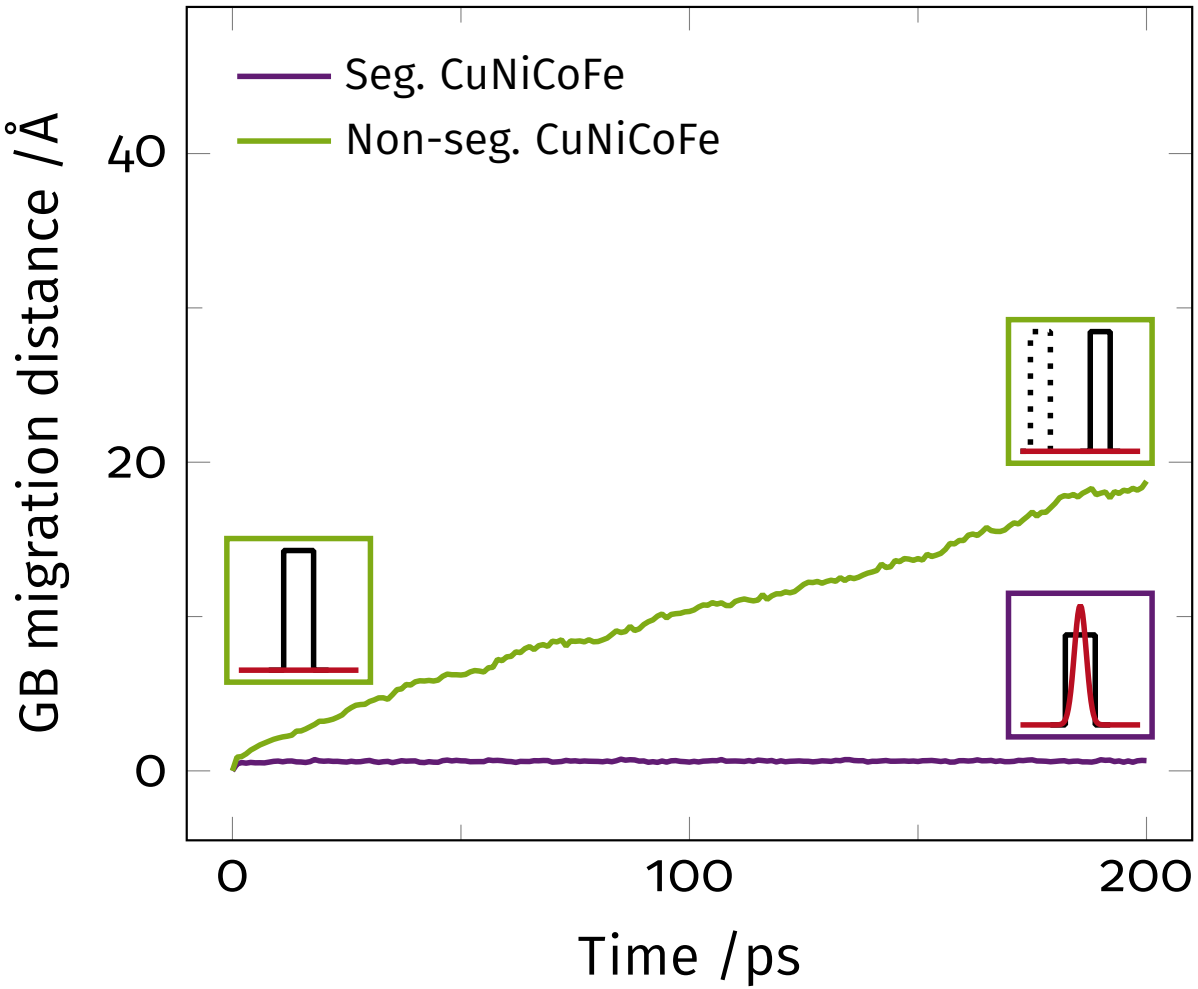

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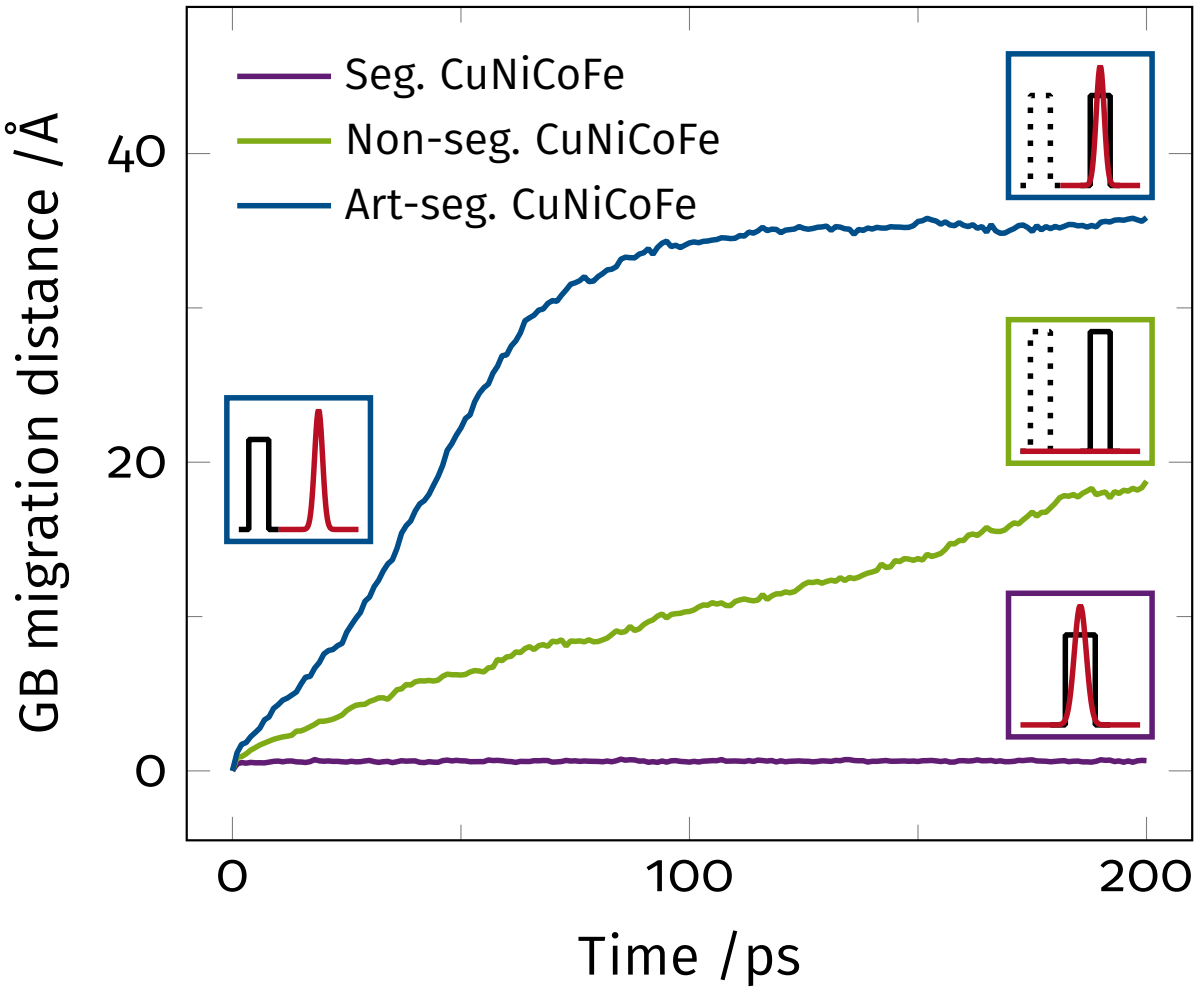
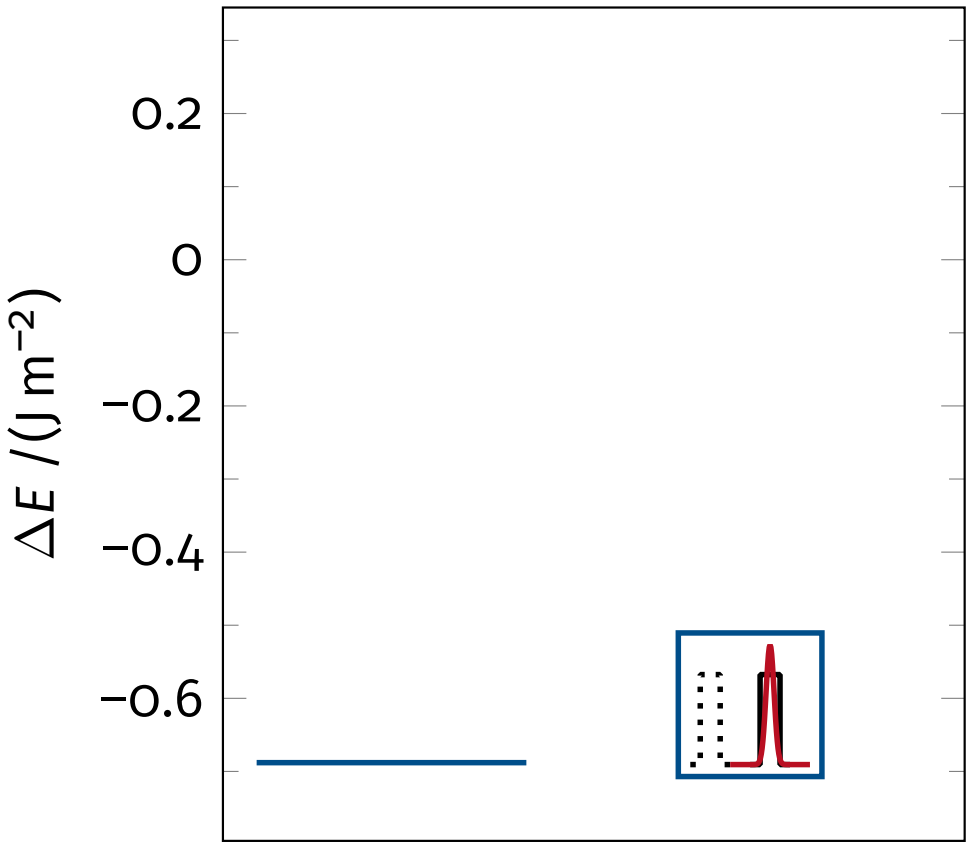


Pinning Energy in the HEA

TECHNISCHE UNIVERSITÄT DARMSTADT

- T = 1200 K
- $\Delta E = (E_{\text{final}} - E_{\text{initial}})/A_{\text{GB}}$



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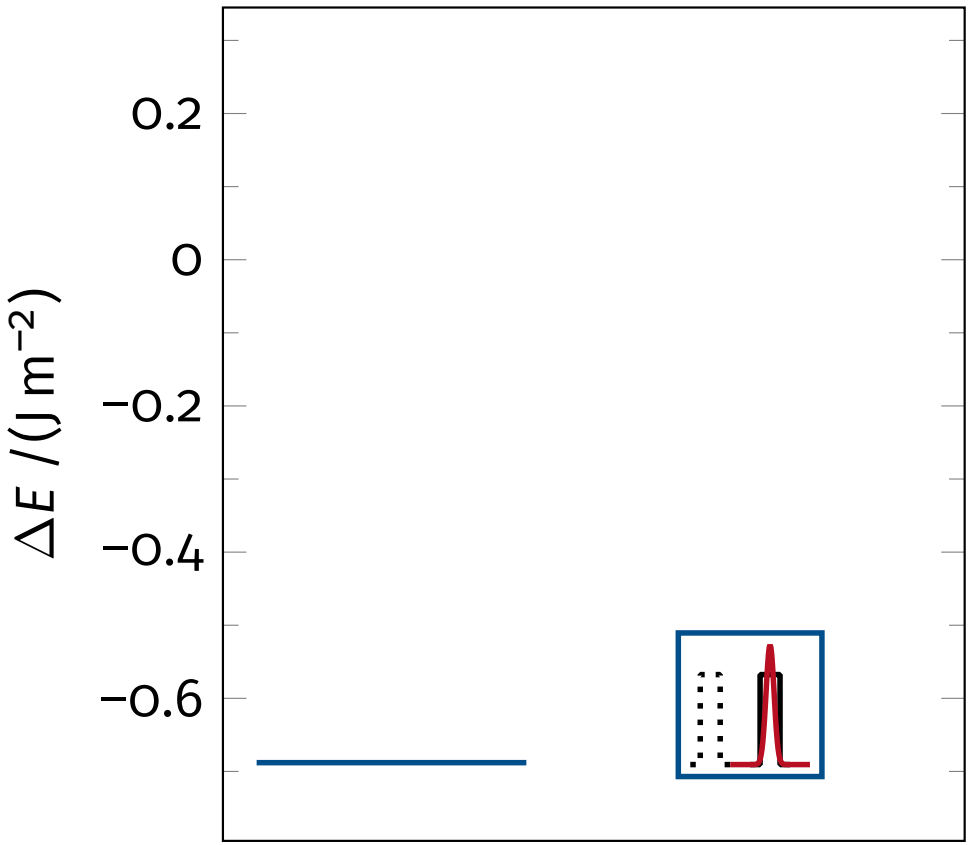
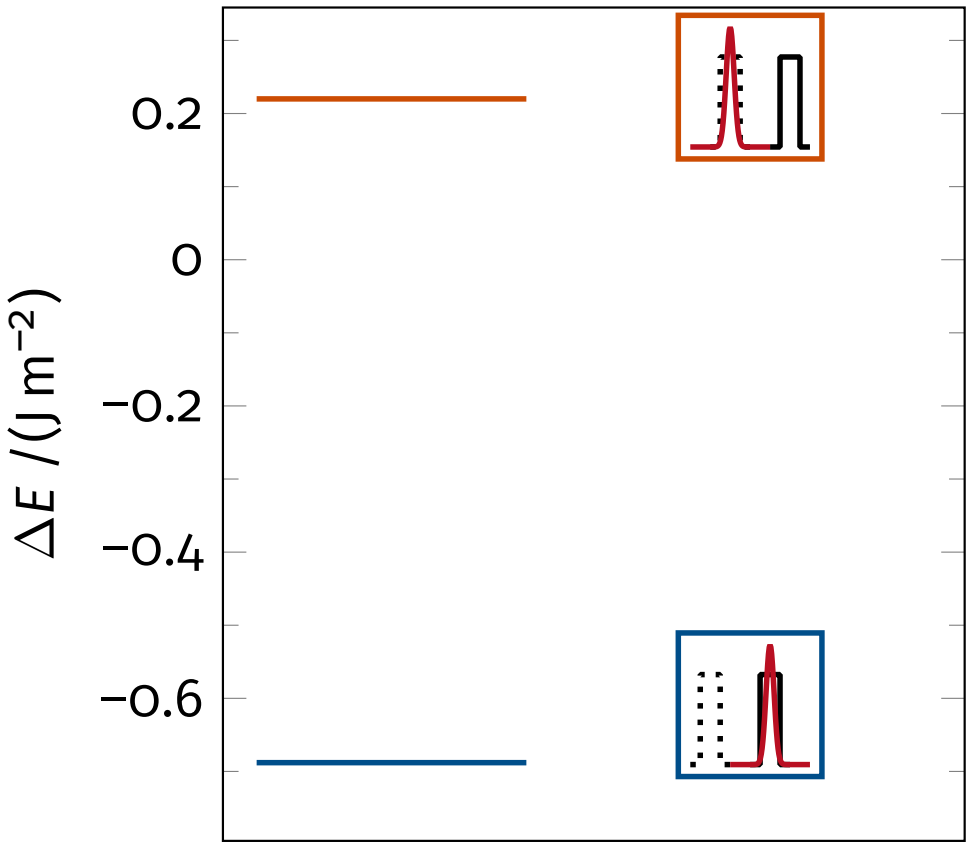


- Inserted Cu layer strongly attracts the STGB.

Pinning Energy in the HEA

TECHNISCHE UNIVERSITÄT DARMSTADT

- T = 1200 K
- $\Delta E = (E_{\text{final}} - E_{\text{initial}})/A_{\text{GB}}$
- Very high driving force (Δe = 0.1 eV/atom) to separate GB and solute cloud.
- Inserted Cu layer strongly attracts the STGB.



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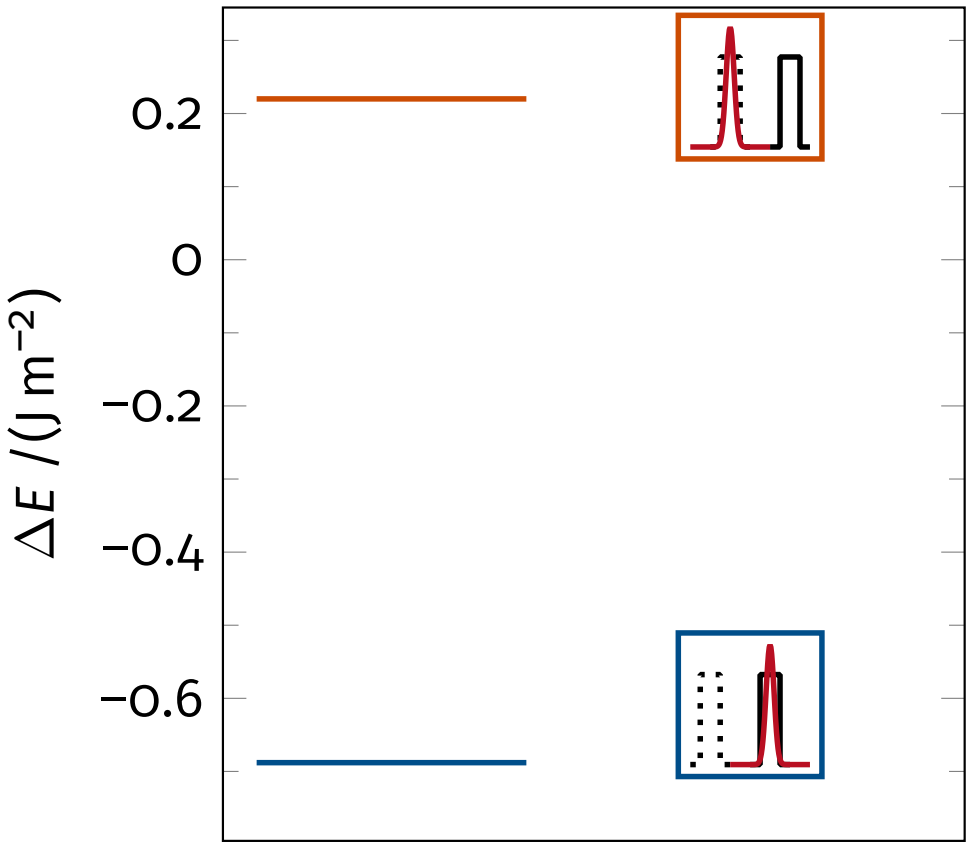
- Inserted Cu layer strongly attracts the STGB.
- GB segregation strongly reduces the GB energy and thereby pins the boundary.



Conclusion

TECHNISCHE UNIVERSITÄT DARMSTADT

- Solute strengthening in the FCC HEA is described well by the Varvenne-Curtin model.

Poster: “Structure and Mobility of Grain Boundaries in High Entropy Alloys: A Molecular Dynamics Study”

Conclusion

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