Grain Boundary Effects in High Entropy Alloys: Insights from Atomistic Computer Simulations

D. Utt, A. Stukowski, K. Albe

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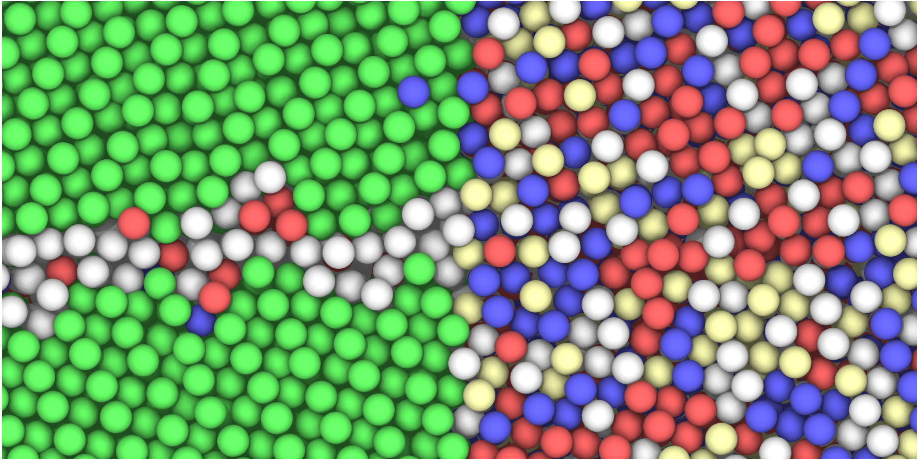
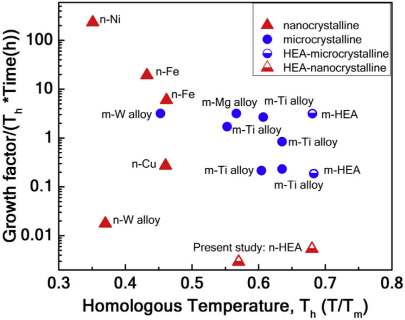


Motivation

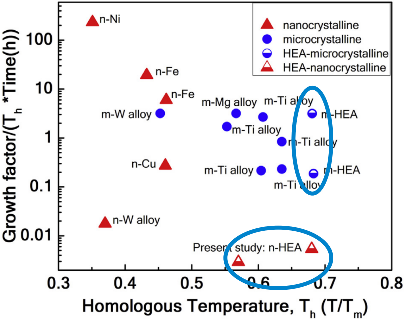
- Growth factor: d_f / d_O



Praveen *et al.*, J. Alloy. Comp., 2016, 662

Motivation

- Growth factor: d_f / d_0
- HEA grain growth factor very small



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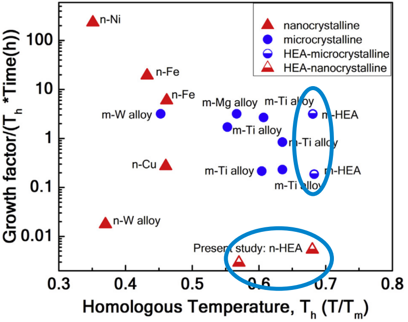

Praveen *et al.*, J. Alloy. Comp., 2016, 662

Motivation

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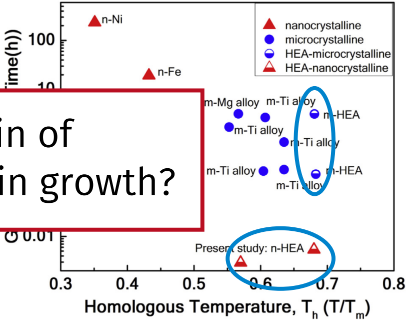
- HEA grain gr small
- Hall-Petch law

What is the origin of the reduced grain growth?



Praveen *et al.*, J. Alloy. Comp., 2016, 662

Possible Causes for Reduced Grain Growth

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- Zener pinning on carbides or oxides

Zou *et al.*, Nano Lett., 2017, 17 (3)
Praveen *et al.*, J. Alloy. Comp., 2016, 662

Possible Causes for Reduced Grain Growth

- Zener pinning on carbides or oxides
- Reduced GB mobility caused by solute drag

Liu *et al.*, Scr. Mater., 2013, 68

Possible Causes for Reduced Grain Growth

- Zener pinning on carbides or oxides
- Reduced GB mobility caused by solute drag
- Reduced driving force due to GB segregation

Zhou *et al.*, Scr. Mater., 2016, 124

Possible Causes for Reduced Grain Growth

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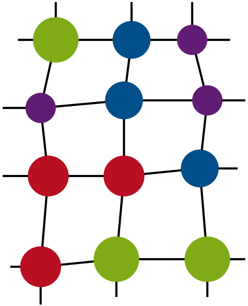
- Zener pinning on carbides or oxides
- Reduced GB mobility caused by solute drag
- Reduced driving force due to GB segregation
- Local lattice distortions



Methodology

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- Atomistic simulations using LAMMPS

www.lammps.sandia.gov

Methodology

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- Atomistic simulations using LAMMPS
- Equimolar FCC CuNiCoFe HEA
    - Random configuration (Rand. ...)
    - Chemical equilibration using hybrid VC-SGC MC/MD

Sadigh *et al.*, Phys. Rev. B, 2012, 85
Koch *et al.*, JAP, 2017, 122

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Zhou *et al.*, Phys. Rev. B, 2004, 69
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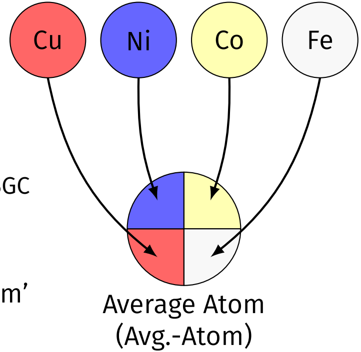

Varvenne *et al.*, Phys. Rev. B, 2016, 93

Lattice Distortions

What is the magnitude of the intrinsic lattice distortions?

Lattice Distortions

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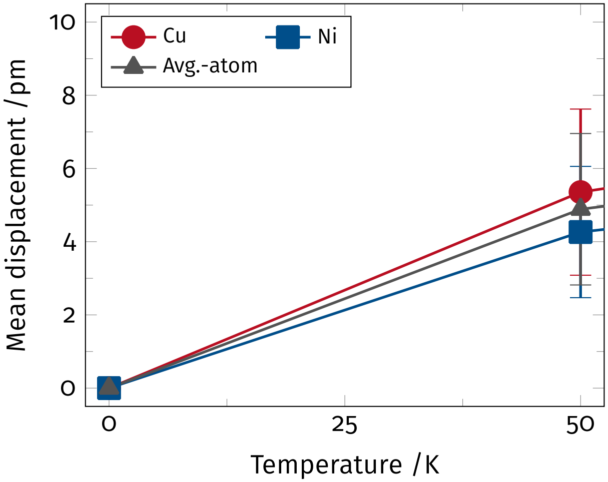
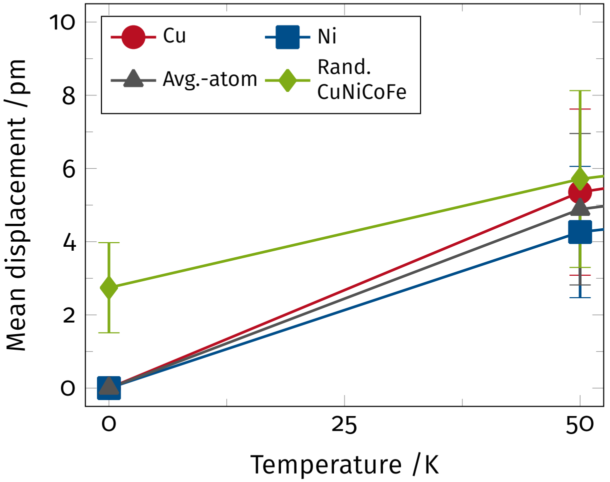


Lattice Distortions



Lattice Distortions

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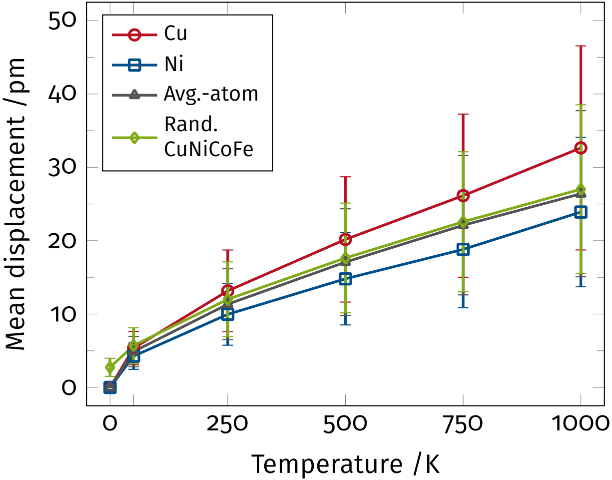
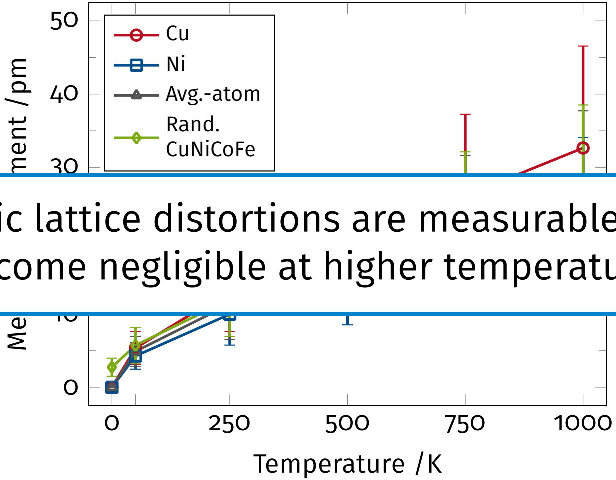


Lattice Distortions



Intrinsic lattice distortions are measurable at 0 K, but become negligible at higher temperatures.

$\Sigma\,11\,(332)\,\langle 110 \rangle$ STGB
0 K Structures

Is there a structural difference for the GBs in the different materials?

$\Sigma\,11\,(332)\,\langle 110\rangle$ STGB
0 K Structures

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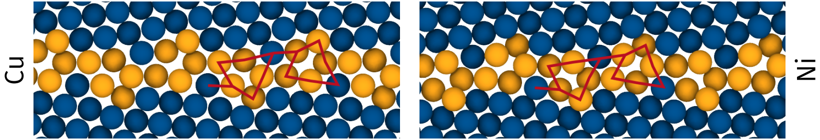
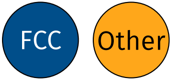
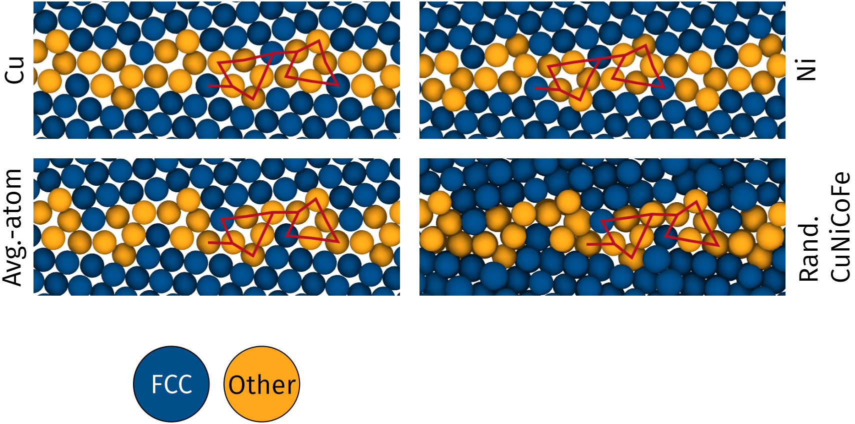




Σ 11 (332) ⟨110⟩ STGB
0 K Structures



Σ 11 (332) $\langle 110 \rangle$ STGB
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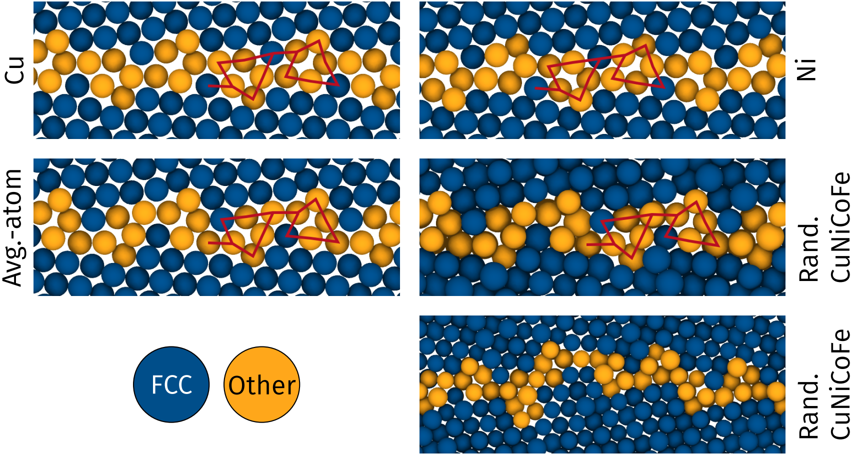

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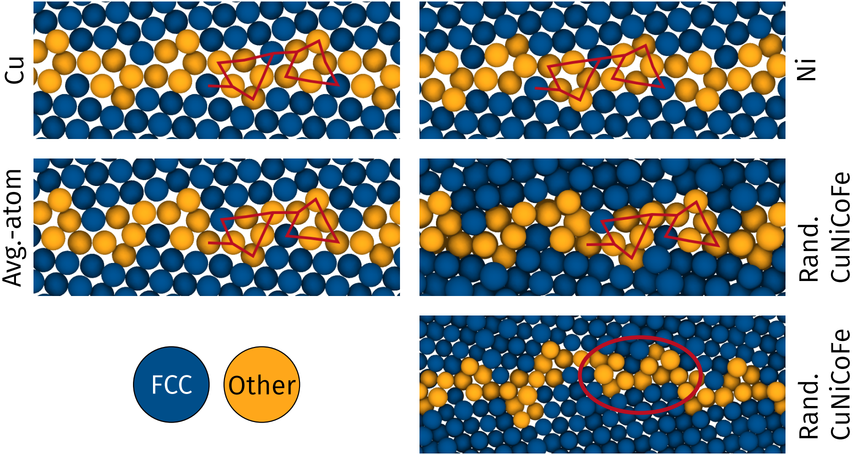

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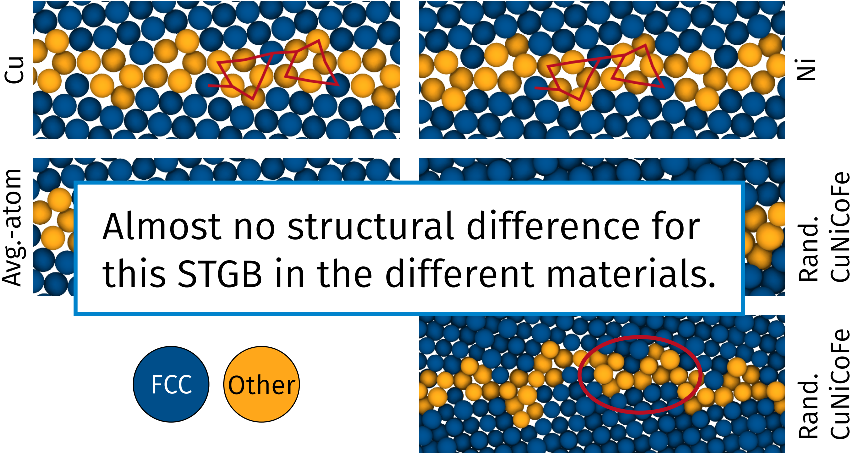

Almost no structural difference for this STGB in the different materials.

Synthetic Driving Force

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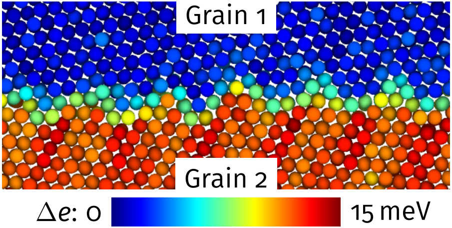
What are the GB mobilities for the different materials under driven conditions?

Synthetic Driving Force



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

Synthetic Driving Force

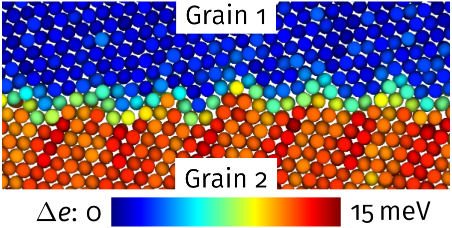
Synthetic driving pressure:

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

GB Mobility:

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

$$M(T) = M^{\infty} \exp\left(\frac{-Q_\mathrm{m}}{k_\mathrm{B}T}\right)$$



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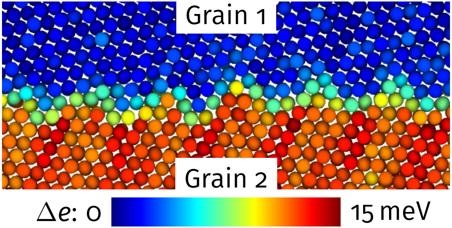
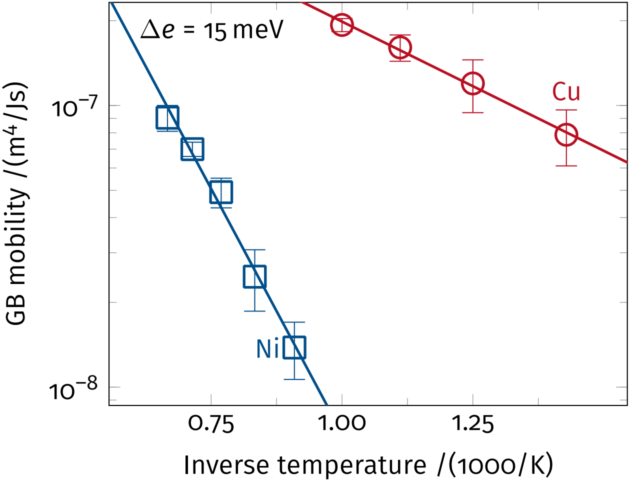


Σ 11 (332) ⟨110⟩ STGB
Mobility



$\Sigma 11\,(332)\,\langle 110 \rangle$ STGB
Mobility

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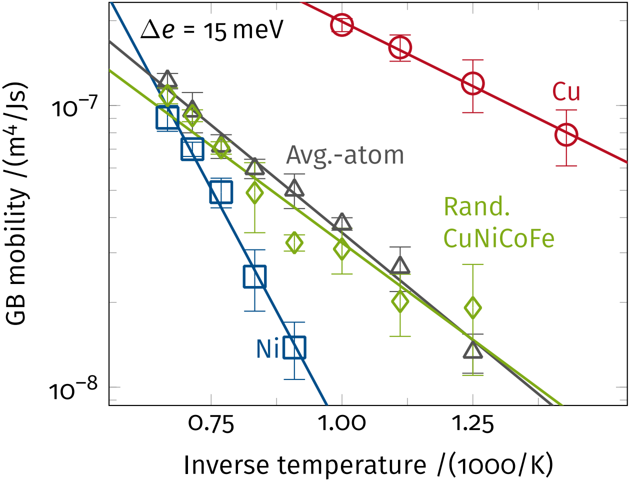

Σ 11 (332) ⟨110⟩ STGB
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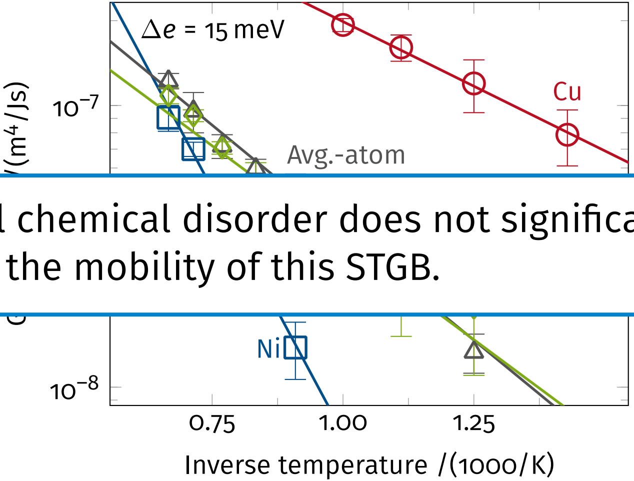

Local chemical disorder does not significantly alter the mobility of this STGB.

Σ 11 (332) ⟨110⟩ **STGB**
Segregation & Mobility

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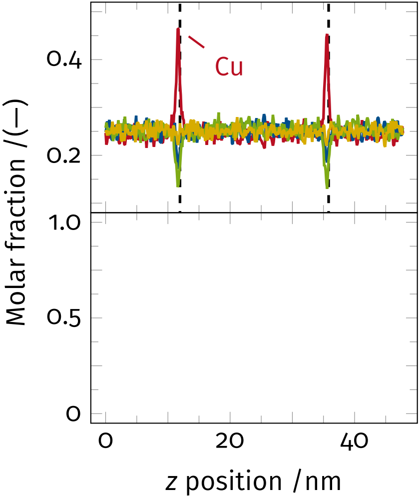
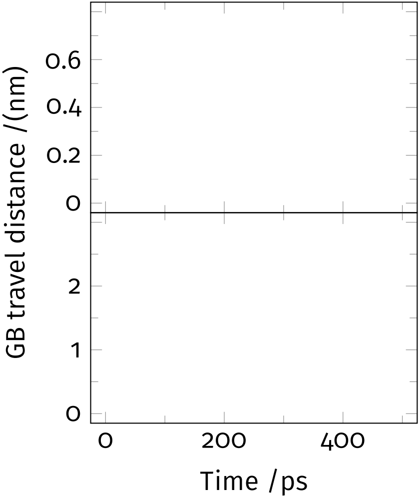
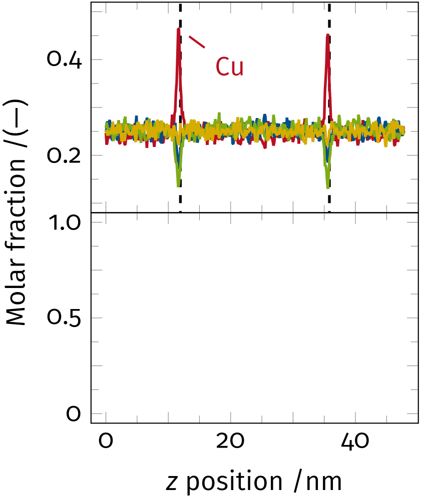
How is the mobility of this STGB altered by segregation?

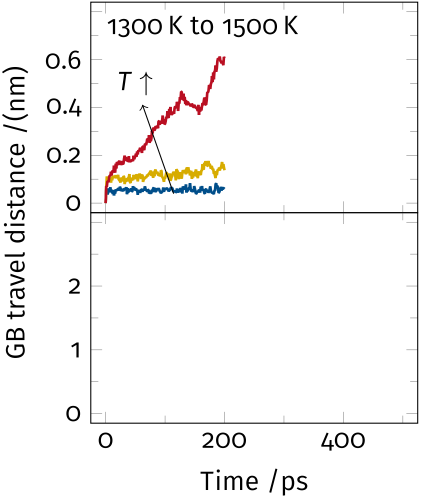
Σ 11 (332) ⟨110⟩ STGB
Segregation & Mobility





Σ 11 (332) ⟨110⟩ STGB
Segregation & Mobility





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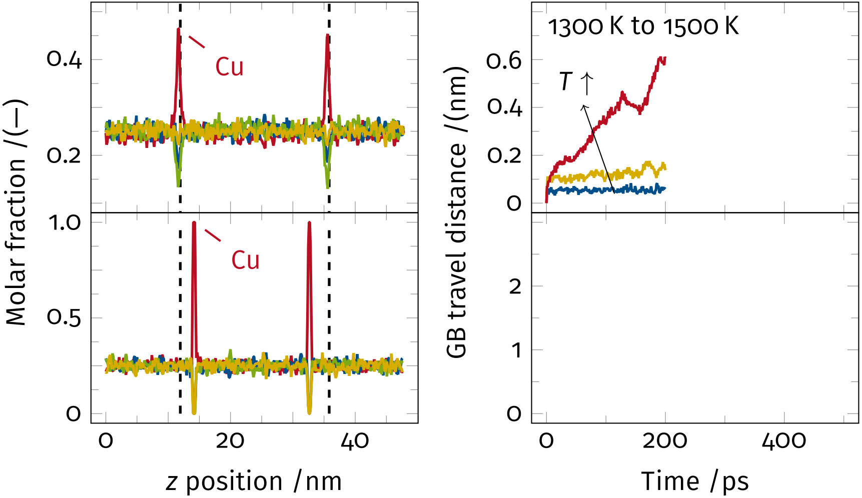

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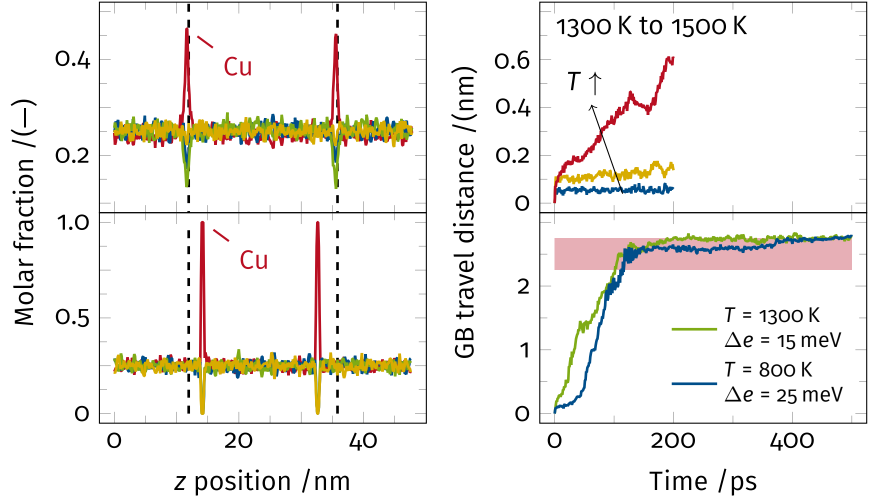

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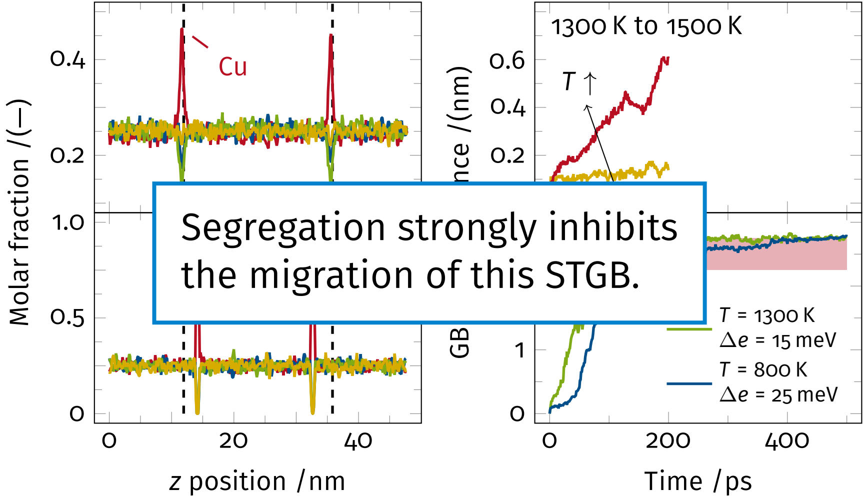
Segregation & Mobility



Segregation strongly inhibits the migration of this STGB.

Nanocrystalline Samples
Expected Grain Growth Rate

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How do these findings transfer to large scale samples containing general GBs?

Nanocrystalline Samples
Expected Grain Growth Rate

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GB velocity:

$$v = M \cdot F$$

Nanocrystalline Samples
Expected Grain Growth Rate

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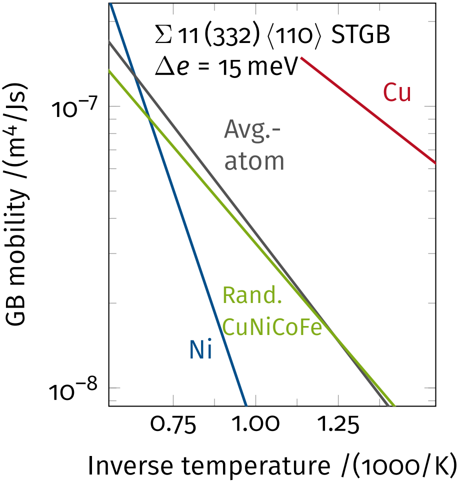

Nanocrystalline Samples
Expected Grain Growth Rate

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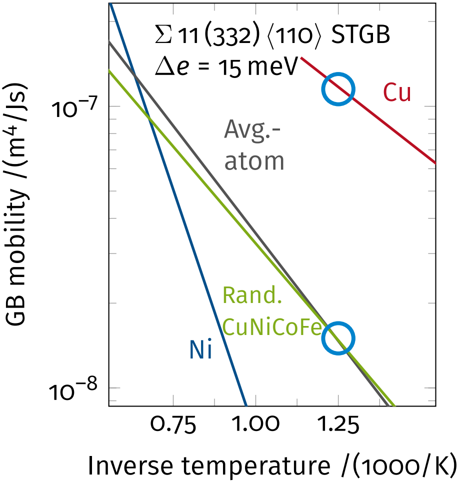

Nanocrystalline Samples
Expected Grain Growth Rate

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Curvature driven GG:

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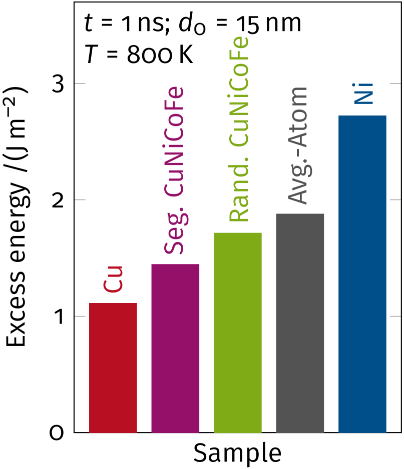

Nanocrystalline Samples
Grain Diameter Evolution

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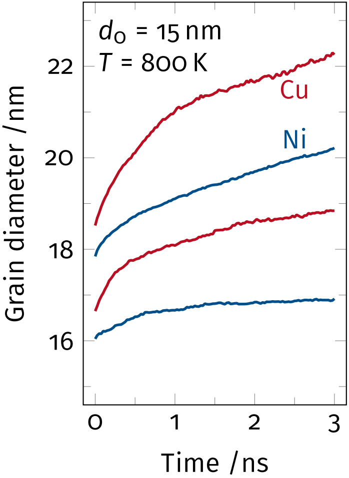

Nanocrystalline Samples
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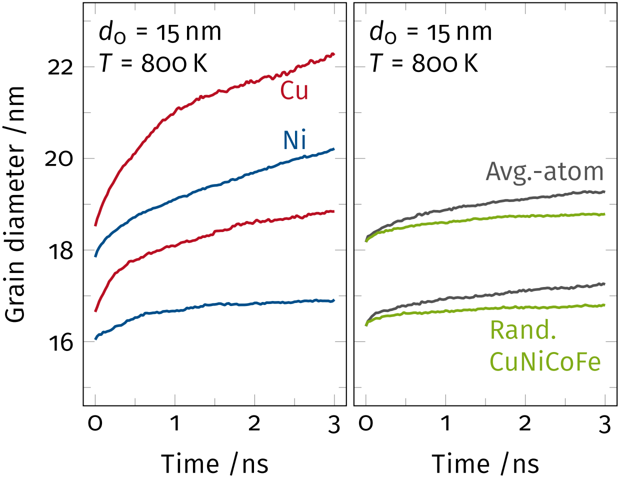

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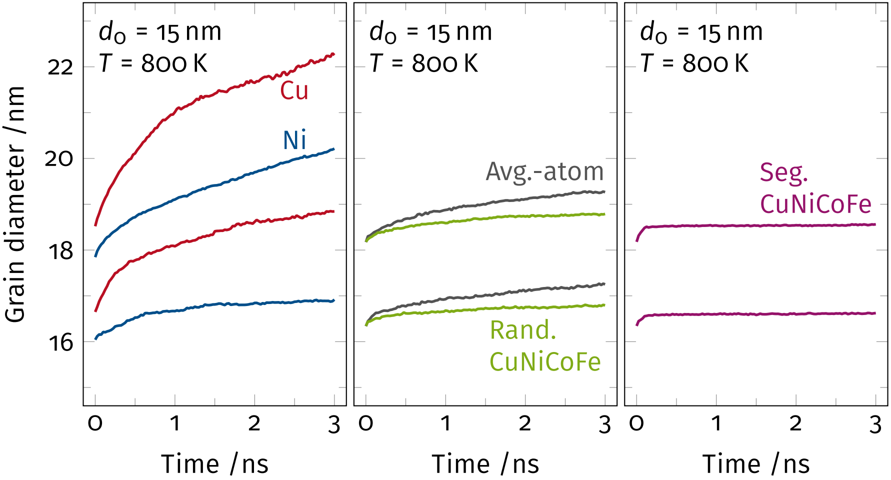

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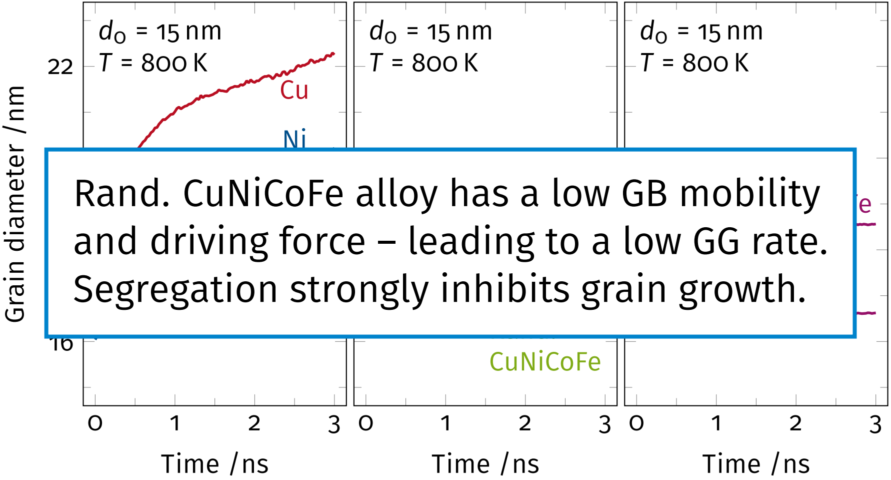

Rand. CuNiCoFe alloy has a low GB mobility and driving force – leading to a low GG rate. Segregation strongly inhibits grain growth.

Summary

- Lattice distortions in the CuNiCoFe HEA are influential at 0 K, but become negligible above 50 K.

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- Avg.-atom and random HEA show almost identical GB mobilities, indicating that the local chemical fluctuations do not hinder GB migration.

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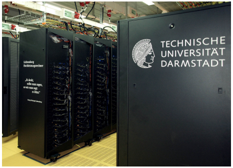
‘Compositionally Complex Alloys – High Entropy Alloys’
SPP 2006; STU 611/2-1



Properties of the avg.-atom

		Rand. CuNiCoFe	Avg. Atom
a_0	(Å)	3.57	3.57
E_{Coh}	(eV)	−4.14	−4.14
C_{11}	(GPa)	172	170
C_{12}	(GPa)	124	120
C_{44}	(GPa)	101	100
α	($\times 10^{-6}$ K^{-1})	21	21
T_{Melt}	(K)	1550	1425
γ_{SF}	(mJ m^{-2})	28.5	27.0
γ_{USF}	(J m^{-2})	126.9	129.7

$\Sigma\,11\,(332)\,\langle 110 \rangle$ STGB
400 K GB Structures

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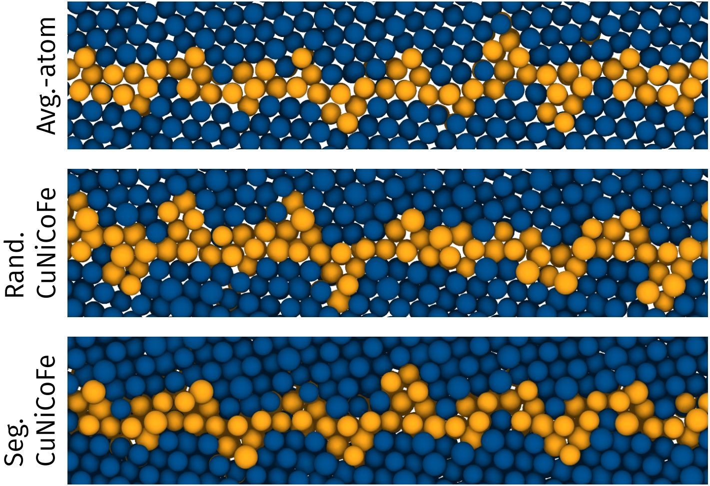

Σ 11 (332) ⟨110⟩ STGB
Position