

# Structure and Mobility of Grain Boundaries in High Entropy Alloys: A Molecular Dynamics Study

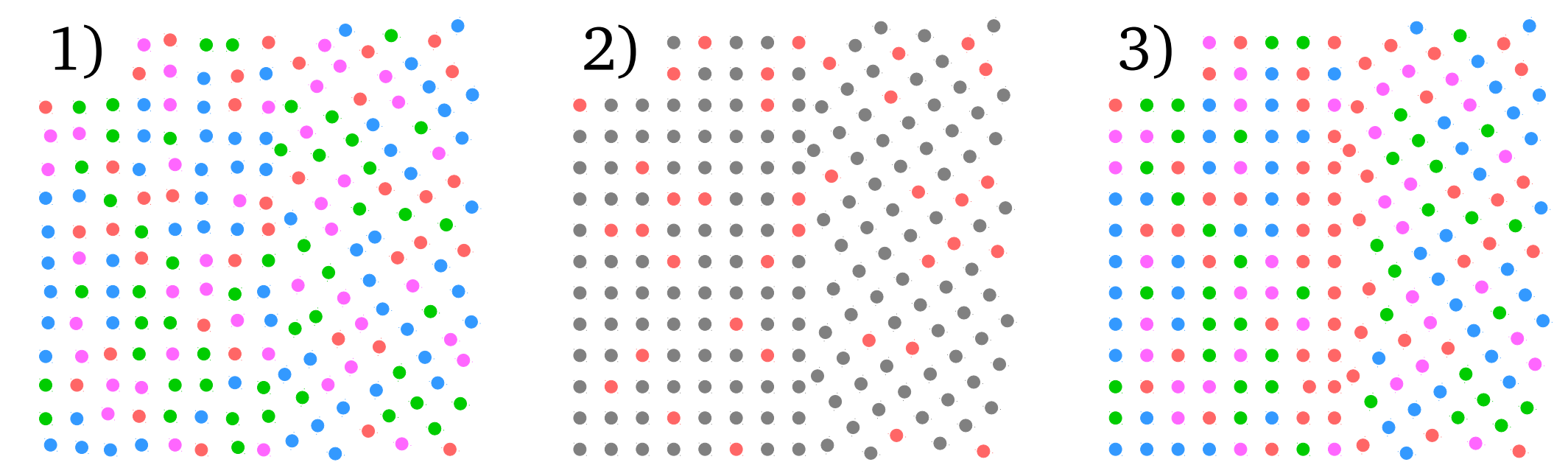


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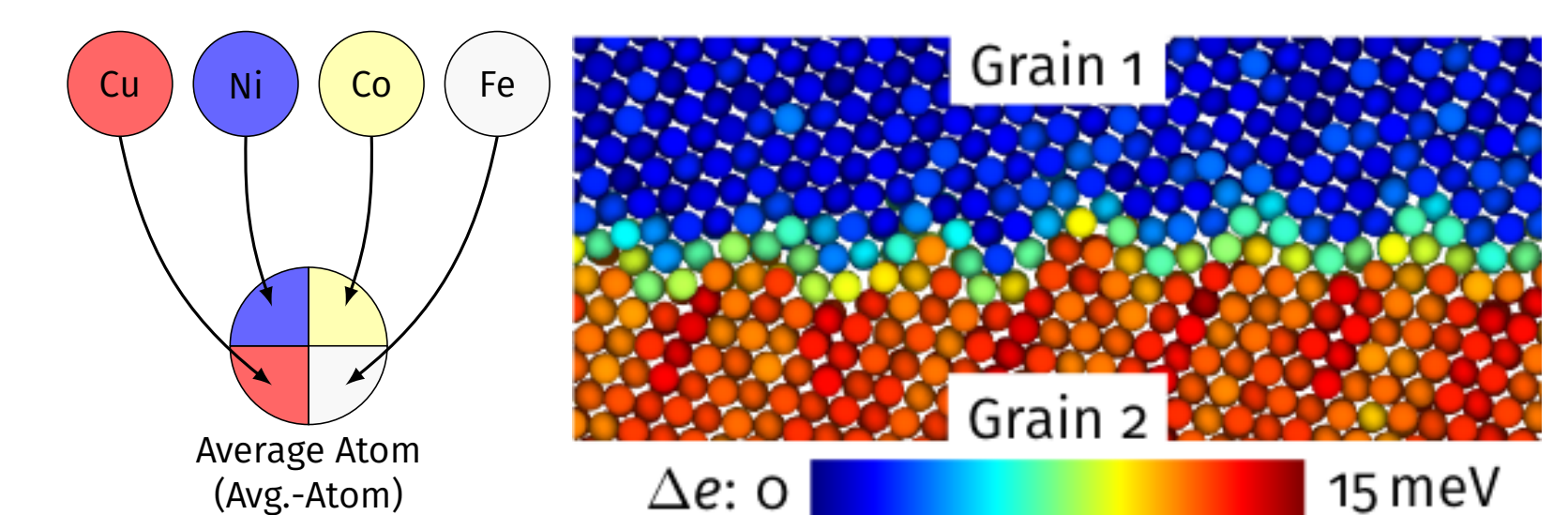
## Motivation

- Reduced grain growth in high entropy alloys (HEAs) has been observed and there are 4 potential reasons:
  - Structural changes at the grain boundaries (GBs) caused by the intrinsic lattice distortions.
  - Solute drag in an average matrix.
  - Solute segregation to the GBs.
  - Secondary phase formation at the GBs.
- We want to determine which one of these is responsible for the reduced grain boundary mobility.



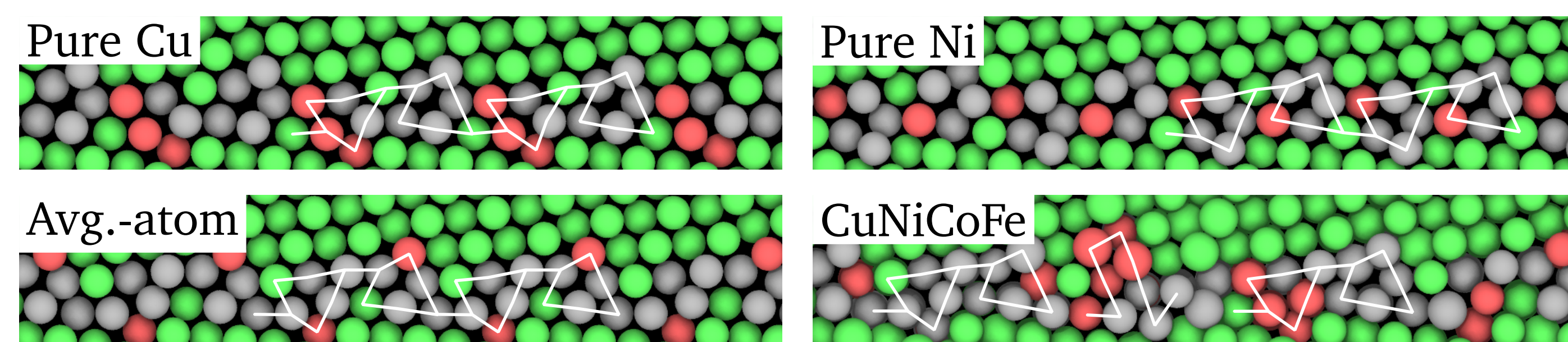
## Computational methods

- $\Sigma 11$  (332)  $\langle 110 \rangle$  symmetrical tilt grain boundary (STGB) in bicrystalline configuration.
- We performed classical molecular dynamics simulations using LAMMPS using embedded atom method (EAM) potentials for the pure metals and the model CuNiCoFe HEA. [1,2]
- We derive an average atom (avg.-atom) potential [3] for the model HEA.
- Migration of the planar STGB driven by a synthetic driving force. [4]
- Solute segregation is simulated using a Monte Carlo algorithm. [5]



## Grain Boundary Structure

Is there a structural difference for the  $\Sigma 11$  STGB in the HEA caused by the intrinsic lattice distortions?  
 $T = 0 \text{ K}$  | •Other | •FCC | •HCP

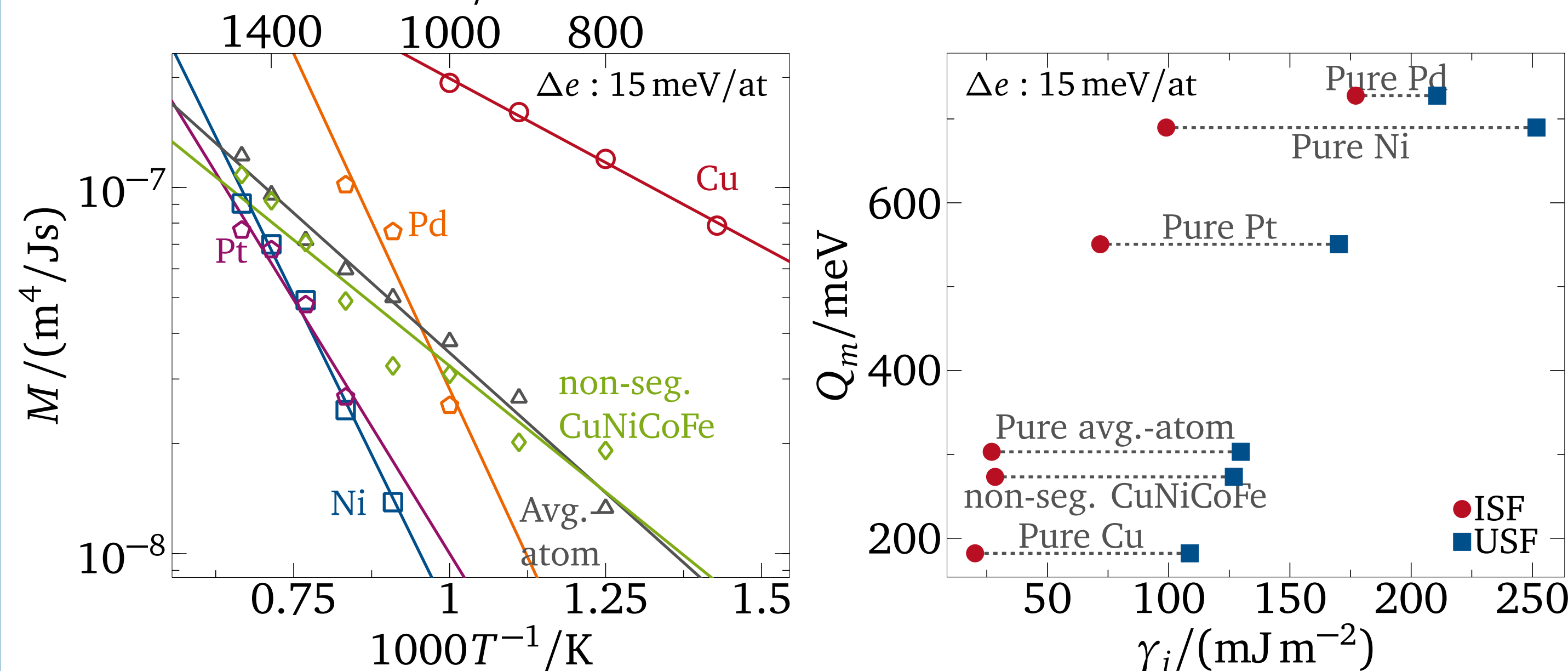


- Almost identical 0 K STGB structures. The repeating structural units for this STGB are marked in white. [6]
- Localized deviation from the ideal configuration in the HEA which could originate from local variations of the stacking fault energy or the intrinsic lattice distortions.

## Synthetic Driving Force

Is the mobility of the  $\Sigma 11$  STGB systematically reduced compared to other FCC metals?

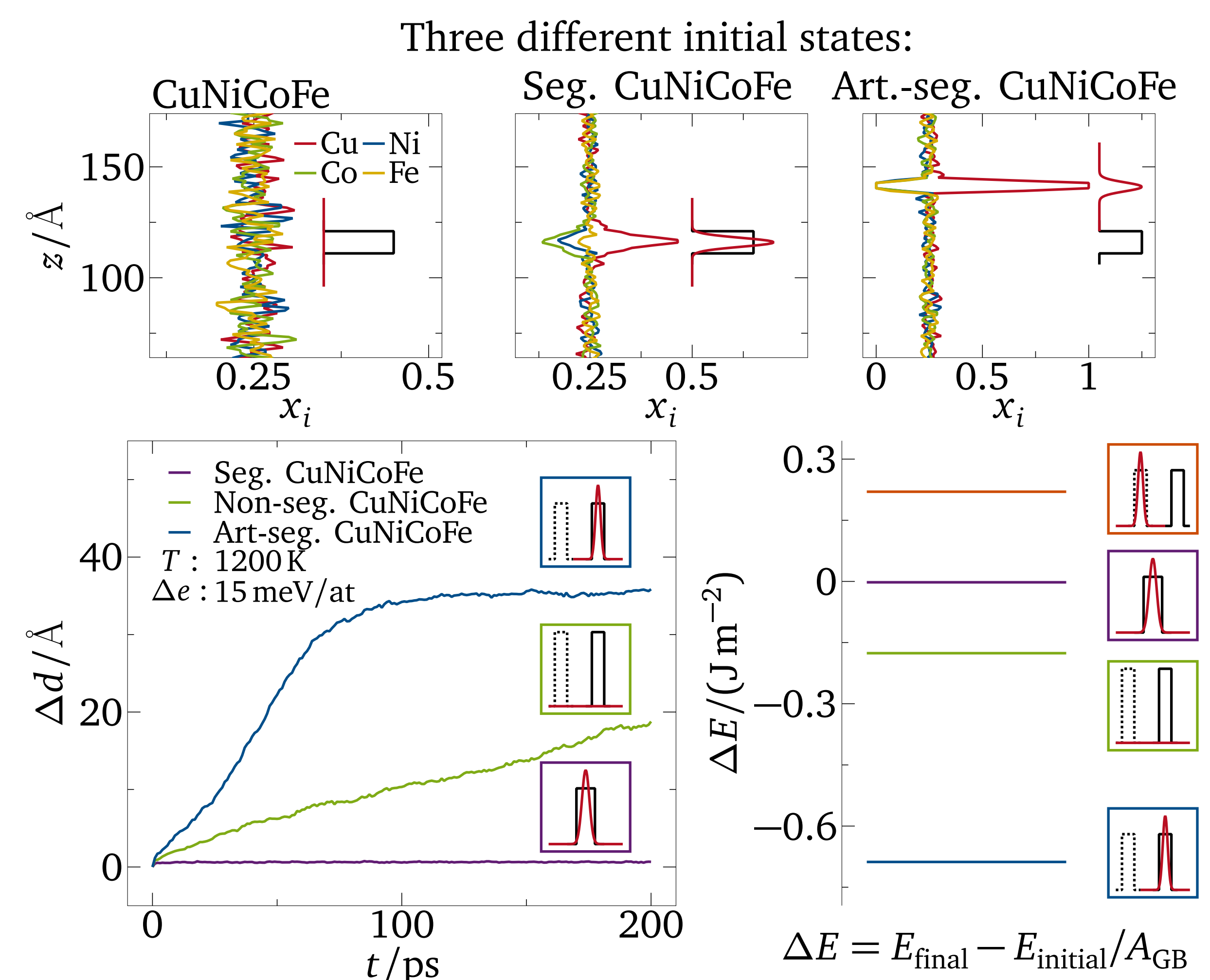
$$P = \frac{\Delta e}{\Omega}, \quad v = M \cdot P, \quad M = M^\infty \exp\left(\frac{-Q_m}{KT}\right)$$



- The HEA does not show a significantly reduced mobility for this  $\Sigma 11$  STGB. Its mobility is almost identical to its average matrix counterpart.
- All samples show a strong correlation between their respective  $\gamma_{ISF}$  and  $\gamma_{USF}$ , and the activation barrier for GB migration. This can be explained by the GB migration mechanism which relies on repeated emission and retraction of Shockley partial dislocations from the GB.

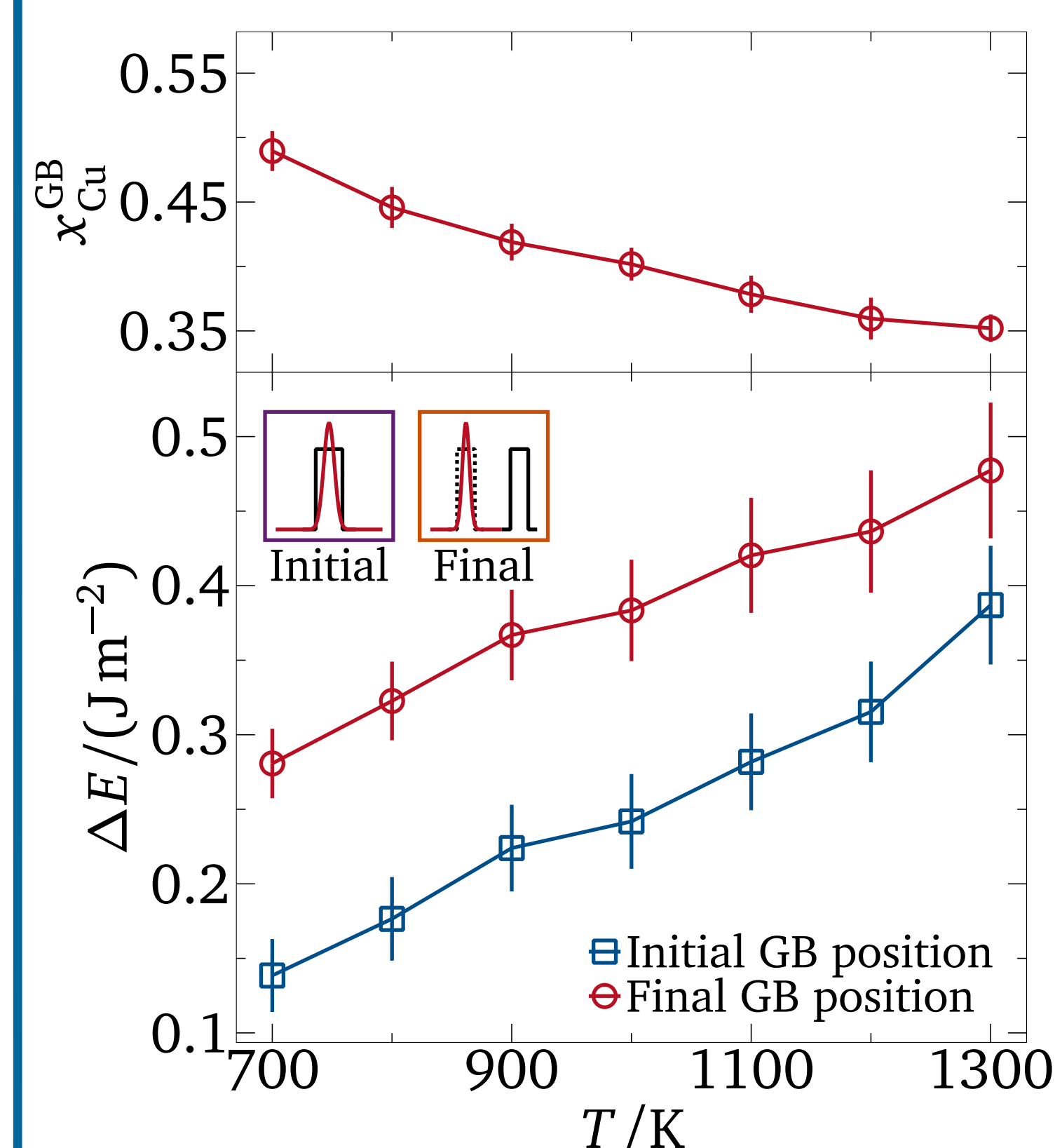
## Grain Boundary Segregation

What is the influence of solute segregation to the  $\Sigma 11$  STGB on its mobility?



- Grain boundary solute segregation pins the  $\Sigma 11$  STGB.
- Cross check: An inserted Cu layer stops the STGB once it is reached.
- The inserted Cu layer strongly attracts the STGB.

How does the pinning energy of the solute cloud scale with temperature?



- We use a driving force of 0.1 eV/at to move the STGB away from the solute cloud.
- $\Delta E = E_{\text{final}} - E_{\text{initial}}/A_{\text{GB}}$
- As the Cu concentration at the STGB decreases, so does the excess energy  $\Delta E$ , which is responsible for the GB pinning.
- The STGB remained stationary at its initial position for the whole temperature range at an synthetic driving force of 0.015 eV/at.