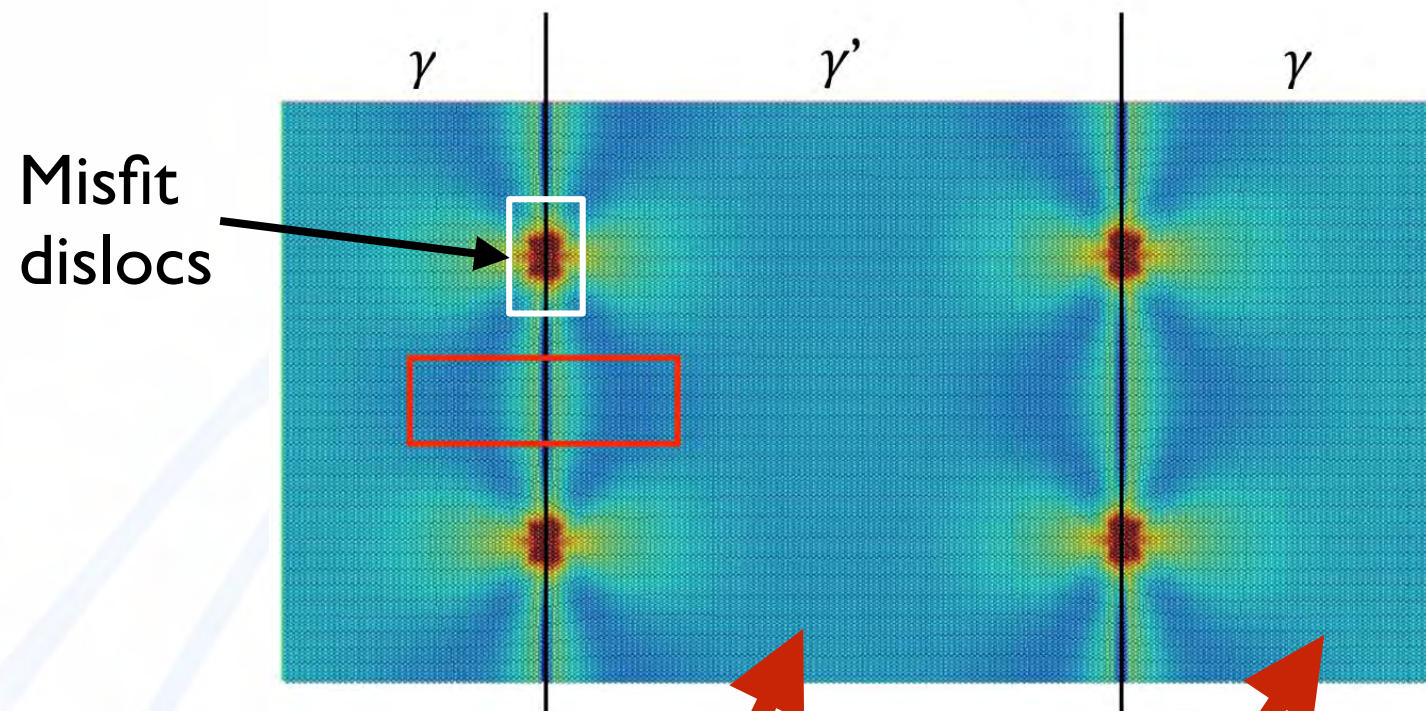
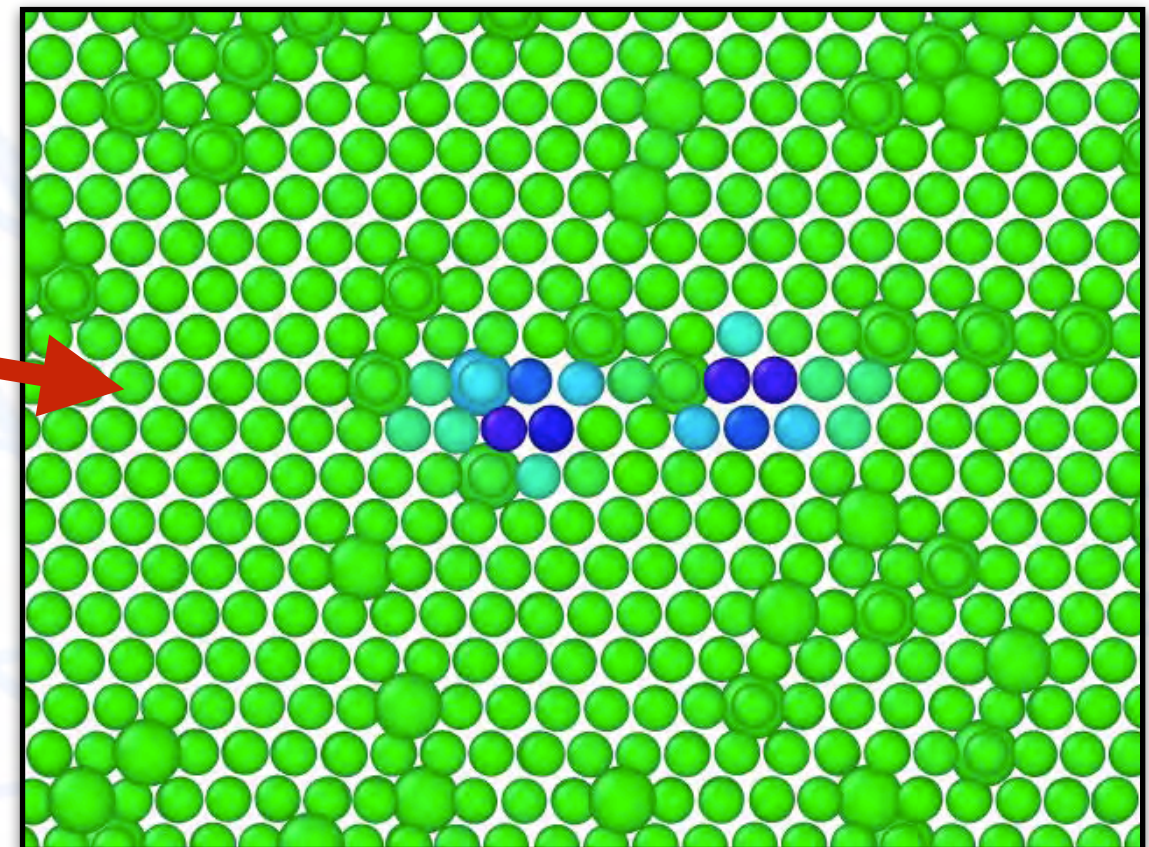
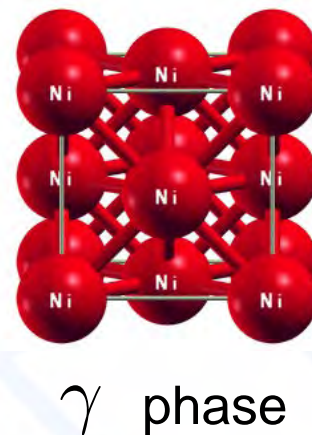
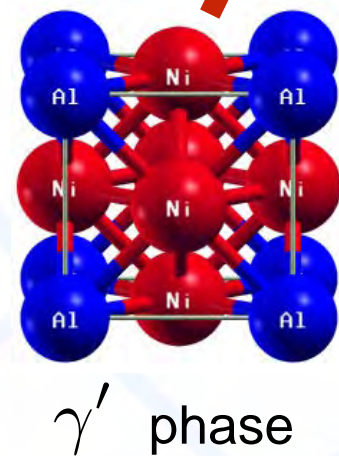


# Example: dislocation glide in Ni-based superalloys



MD simulation of dislocations in  $\gamma$  phase Ni

- Aleatoric and epistemic uncertainties
- Model uncertainty: how accurate is interatomic potential? Parameters and functional form
- Random microstructures, limited data
- Algorithmic uncertainty in solvers
- Limited transferability: can we model chemical complexity, e.g. impurities?



EAM, 5% Al,  $T = 300$  K, 100 MPa shear stress