Phase-field dislocation dynamics modeling of multi-component alloys

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SSGF Program Review

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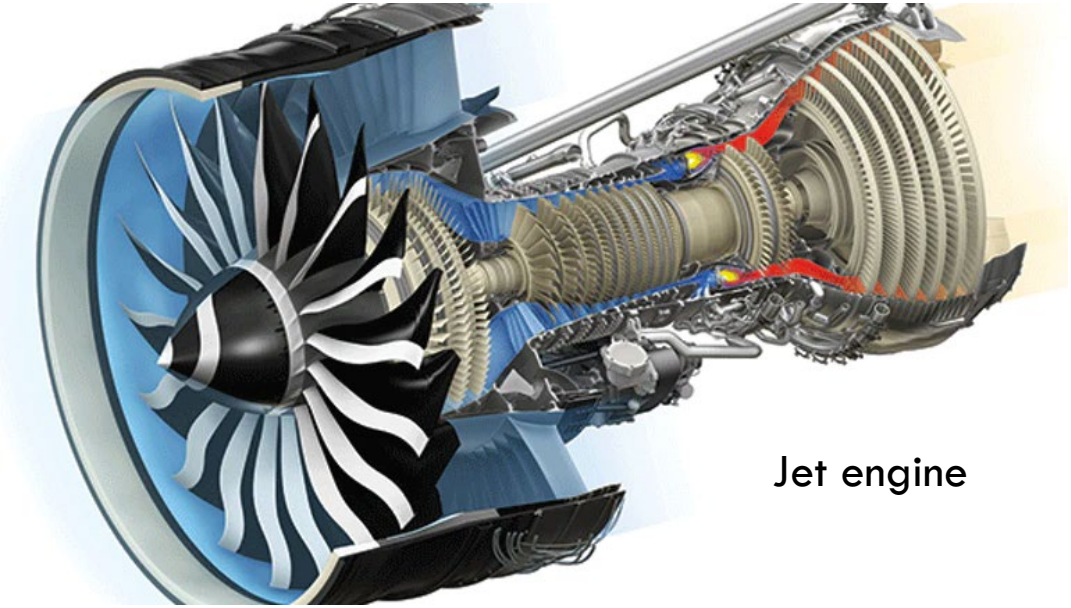
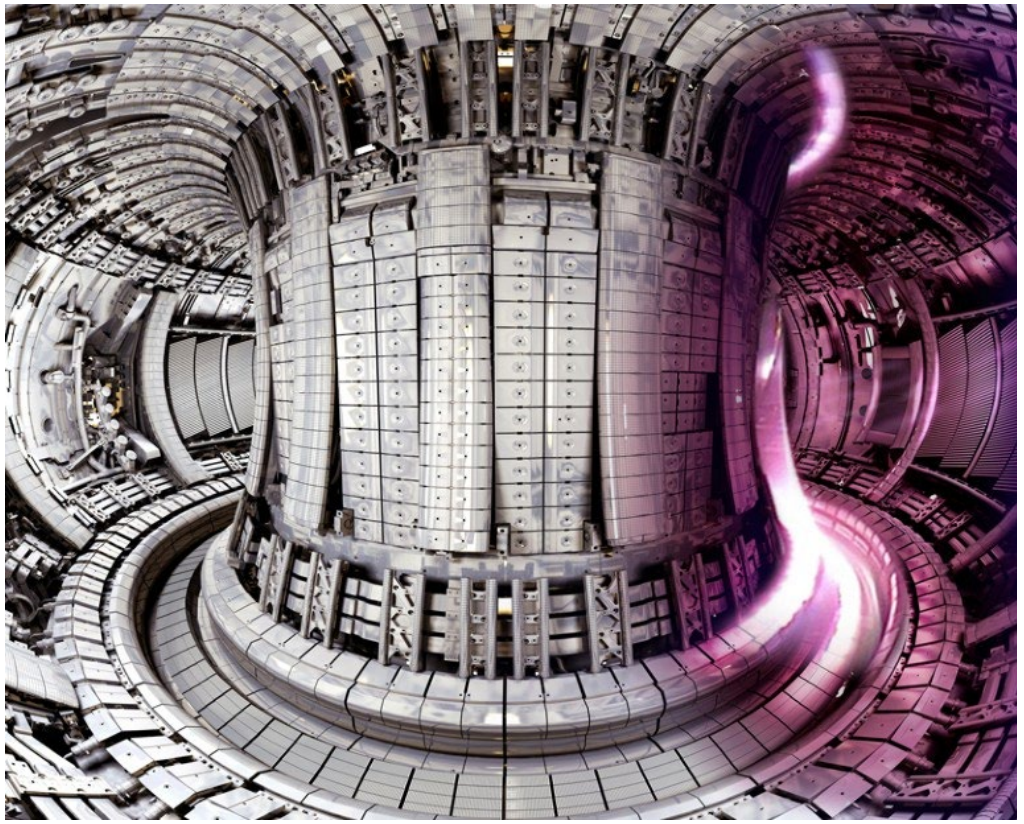
UC SANTA BARBARA

Next-generation materials for extreme environments

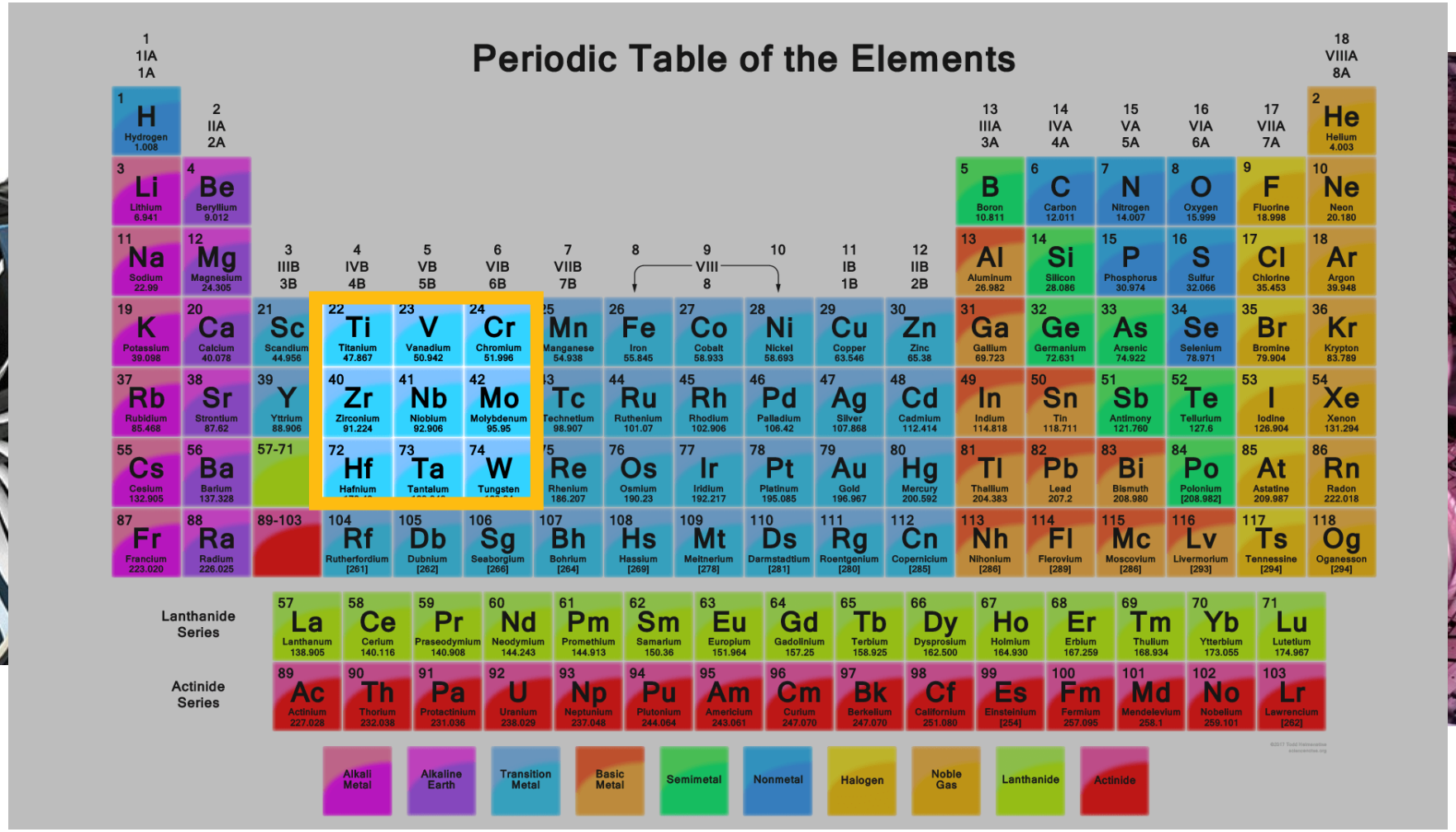


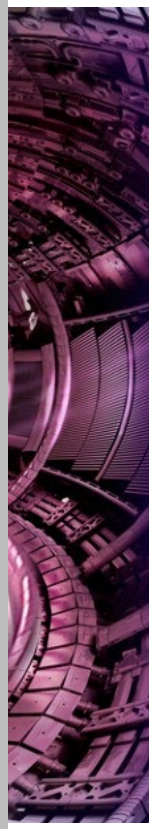
Jet engine



Fusion reactor

Next-generation materials for extreme environments



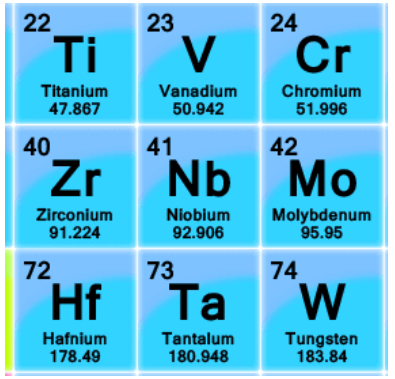


This talk

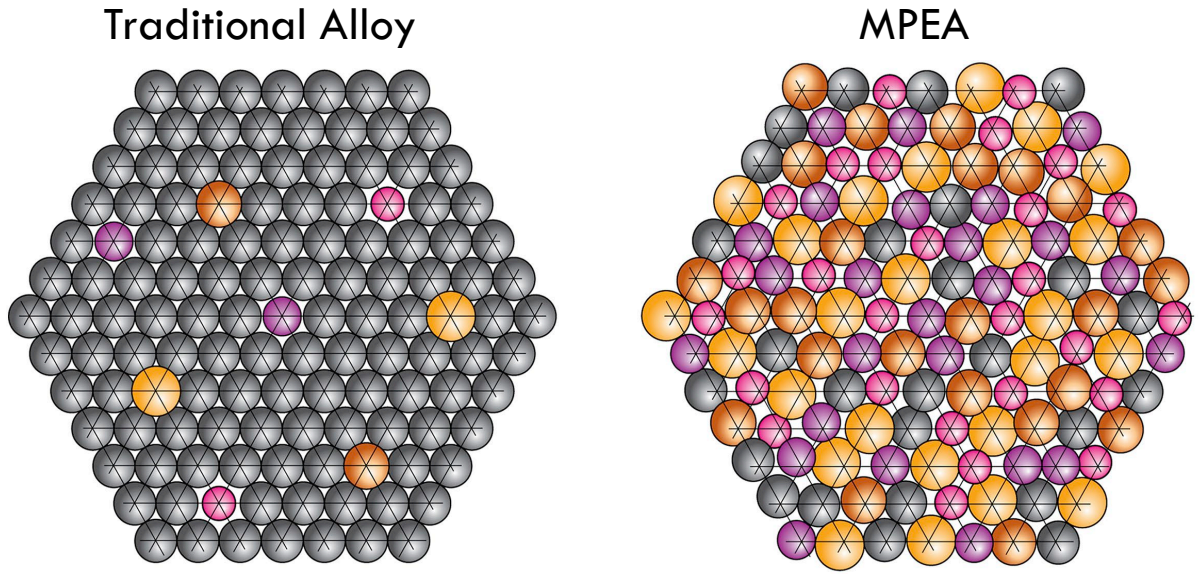
Part I: Refractory Multi-Principal Element Alloys

Part II: Interstitial Elements in Refractory Alloys

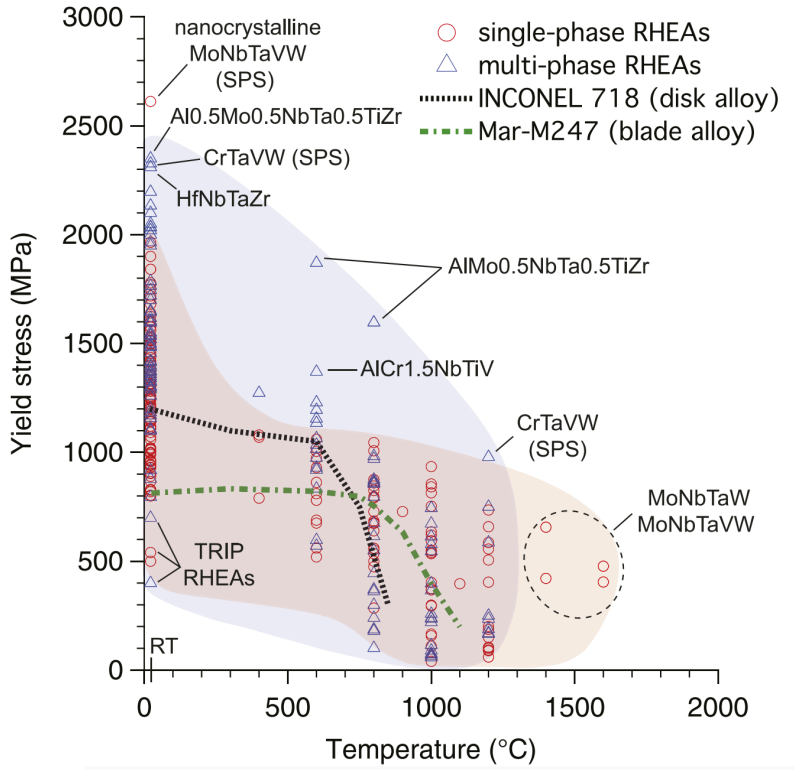
What are multi-principal element alloys?



- Composed of several element types with no dominant species
- Combination of high strength and toughness
- Huge, unexplored composition space



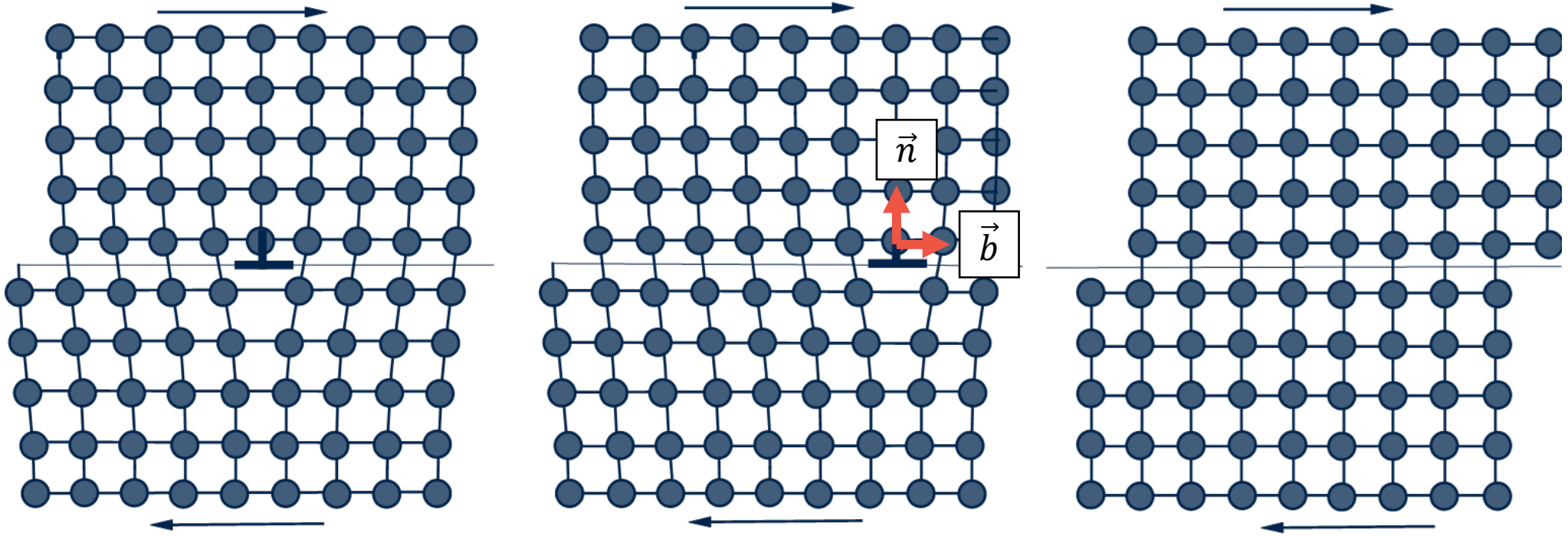
Miracle et al. *Acta Mater*, 122:448-511, 2017.



Senkov, O. N. et al. (2018). J. Mater. Res., 33(19), 3092-3128.

Dislocations control plastic deformation

- Dislocations are defined by their Burgers vector, line direction, and slip plane



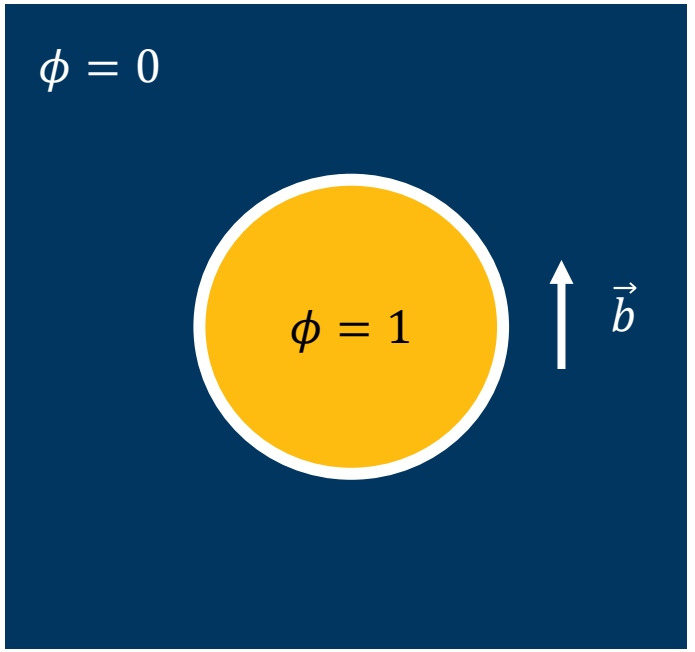
Cai, W., & Nix, W. D. (2016). *Imperfections in Crystalline Solids.*

Screw dislocation: $\vec{b}$ parallel to line direction

Edge dislocation: $\vec{b}$ orthogonal to line direction

Phase-field dislocation dynamics

- Mesoscale, energy-based dislocation model
- Computationally efficient, can run large numbers of simulations
- Uses scalar order parameters (ϕ) to track dislocation structure
  - $\phi = 0$: Unslipped
  - $\phi = 1$: Slipped
  - $0 < \phi < 1$: Dislocation



$$E = E_{elas} + E_{ext} + E_{lattice}$$

Elastic interaction energy

$$E_{elas}(\phi) = \frac{1}{2}[\epsilon - \epsilon^p(\phi)] \cdot C[\epsilon - \epsilon^p(\phi)]$$

$$\epsilon^p(\phi) = \frac{\mathrm{b}\phi}{2\mathrm{d}}(\mathrm{s} \otimes \mathrm{n} + \mathrm{n} \otimes \mathrm{s})$$

Externally applied energy

$$E_{ext}(\phi) = \sigma^{app} \cdot \epsilon^p(\phi)$$

Energy to break bonds (material specific)

$$E_{lattice}(\phi) = \frac{E_{USFE}}{d_{slip}} \sin^2 \pi\phi$$

Phase-field dislocation dynamics

- Mesoscale, energy-based dislocation model
- Computationally efficient, can run large numbers of simulations
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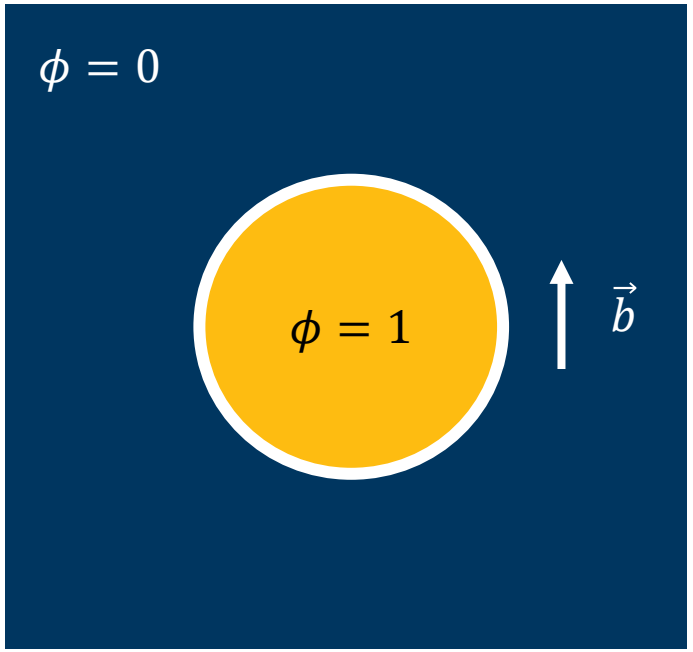


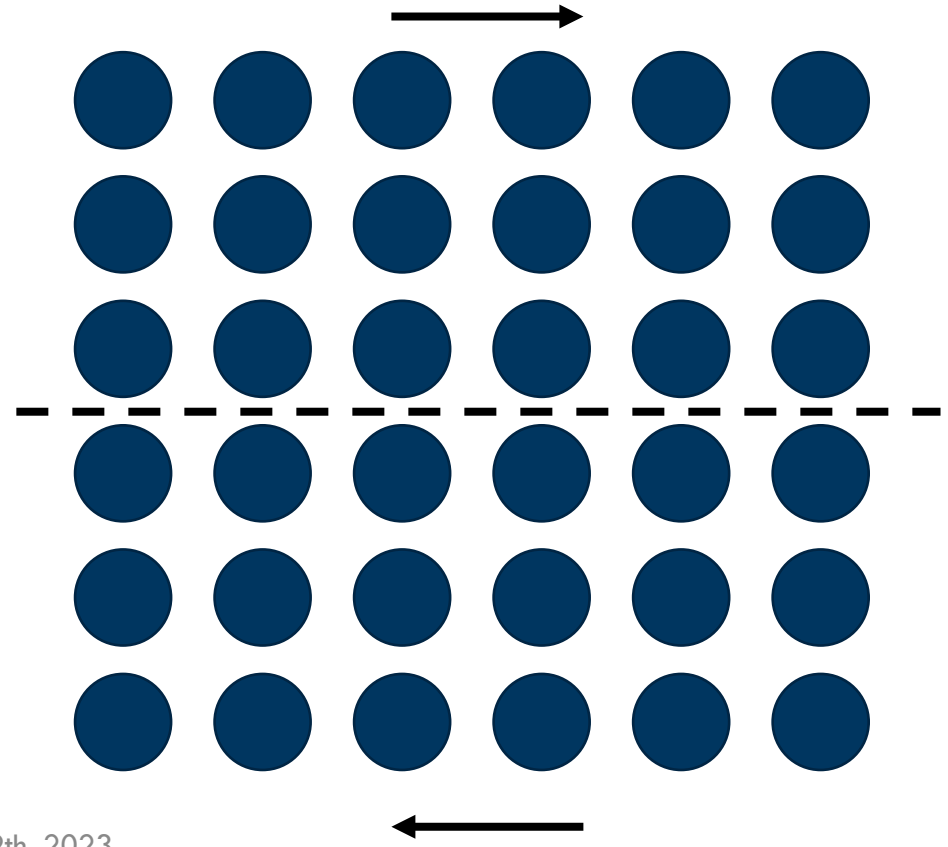
$$E = E_{elas} + E_{ext} + E_{lattice}$$

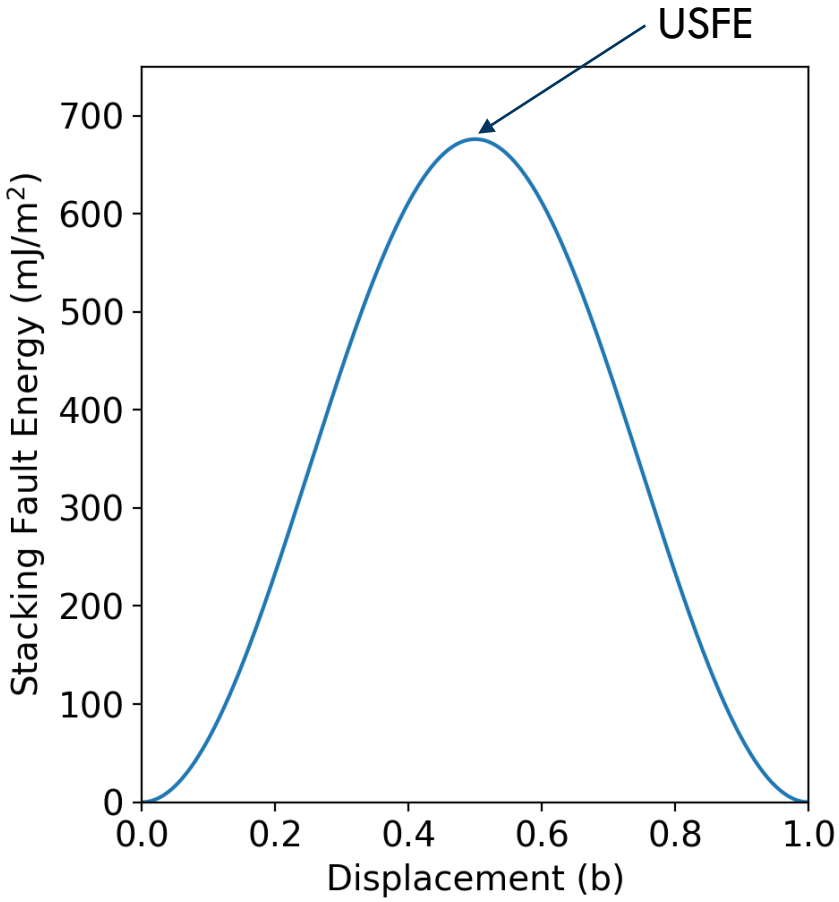
Total energy minimized with Ginzburg-Landau Equation

$$\boxed{\frac{d\phi}{dt} = -m_{disl}\frac{\partial E}{\partial \phi}}$$

Unstable stacking fault energy (USFE)

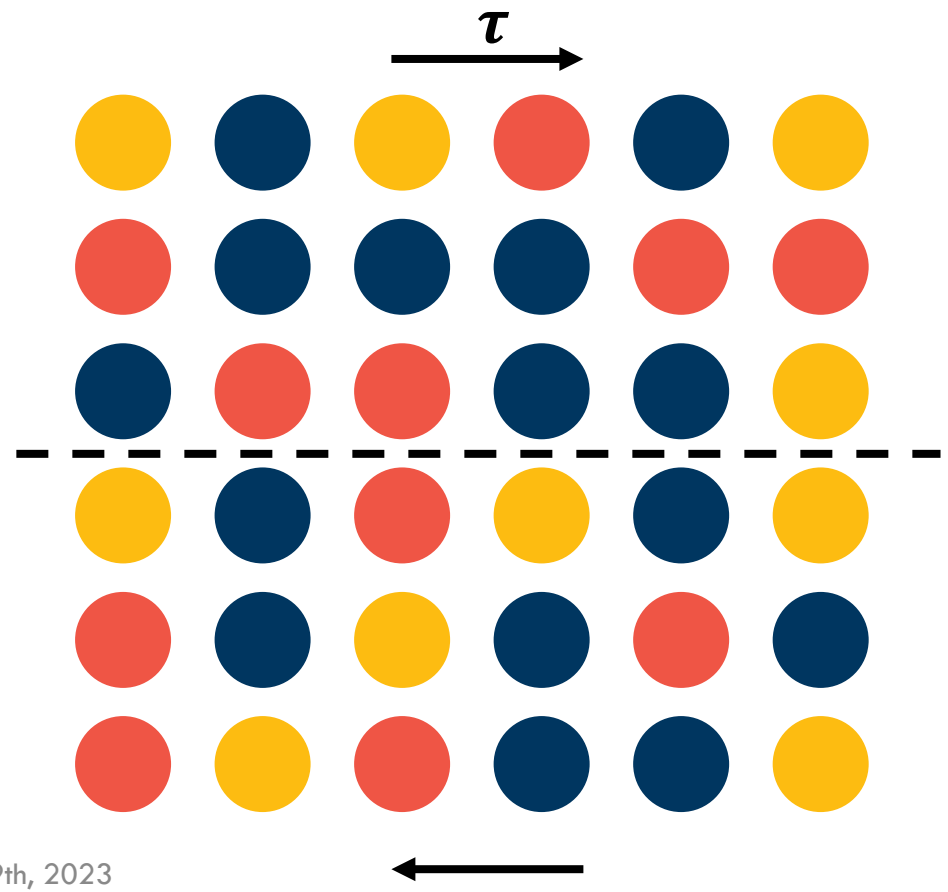
- USFE measures energy required to break bonds across the slip plane
- Used to parameterize lattice energy in PFDD

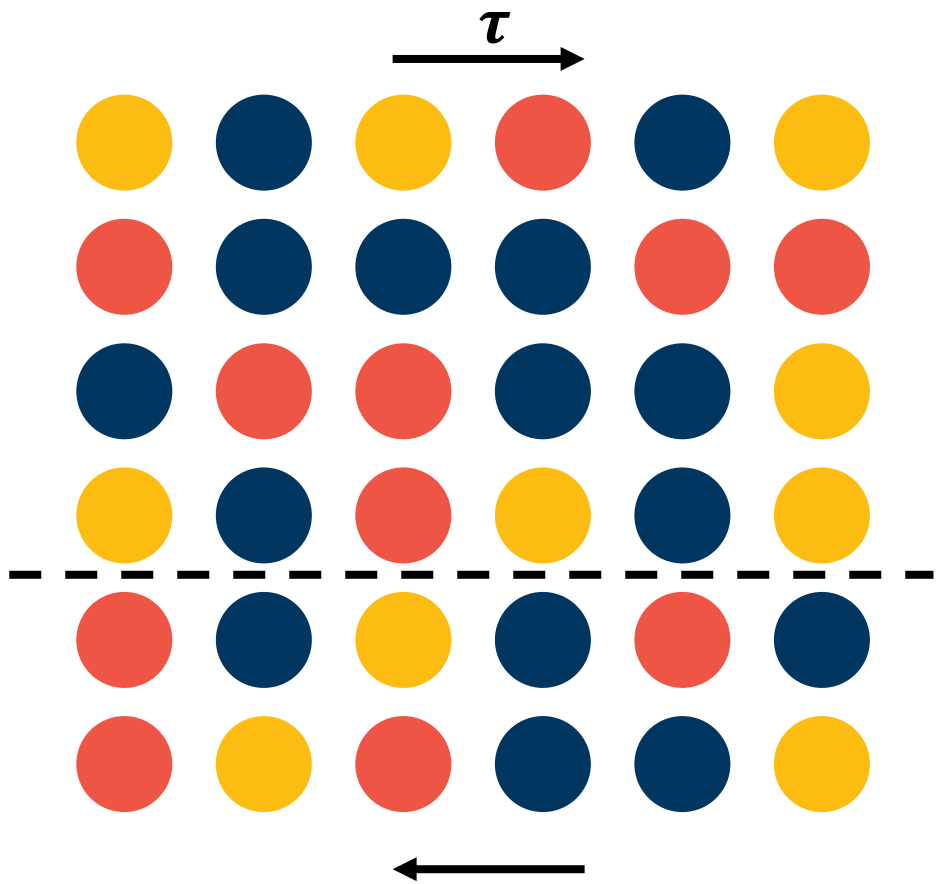




Unstable stacking fault energy in an MPEA

- MPEAs have a disordered lattice
- Local USFE will vary depending on composition and local atomic configurations

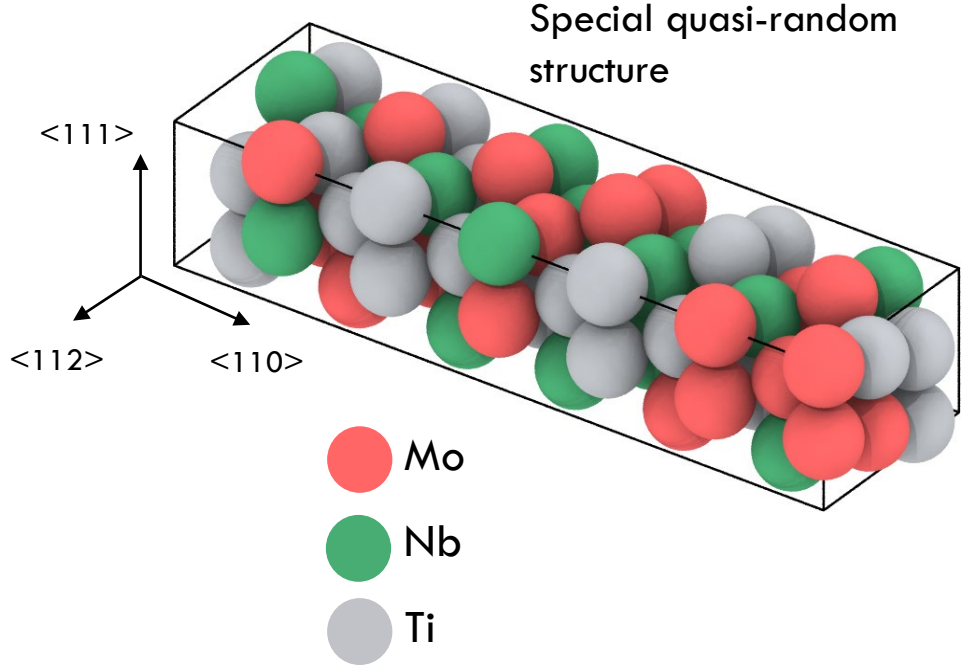


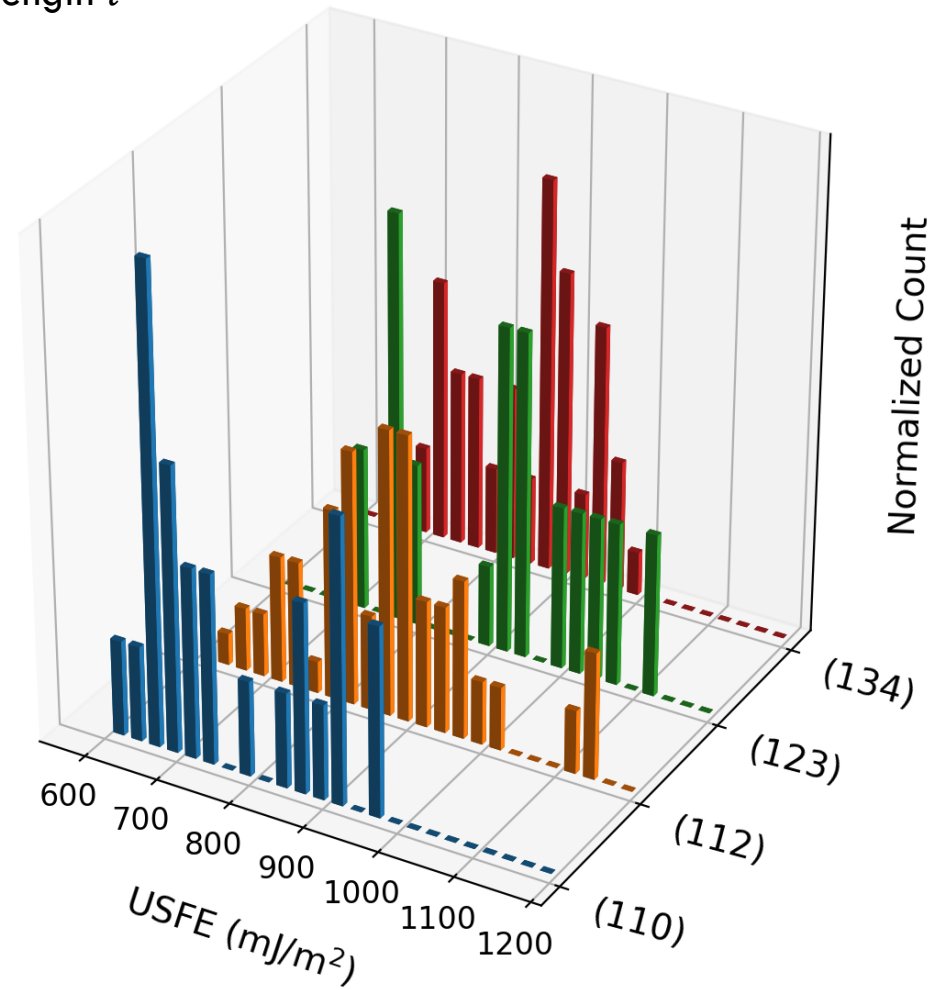


Unstable stacking fault energy – MoNbTi

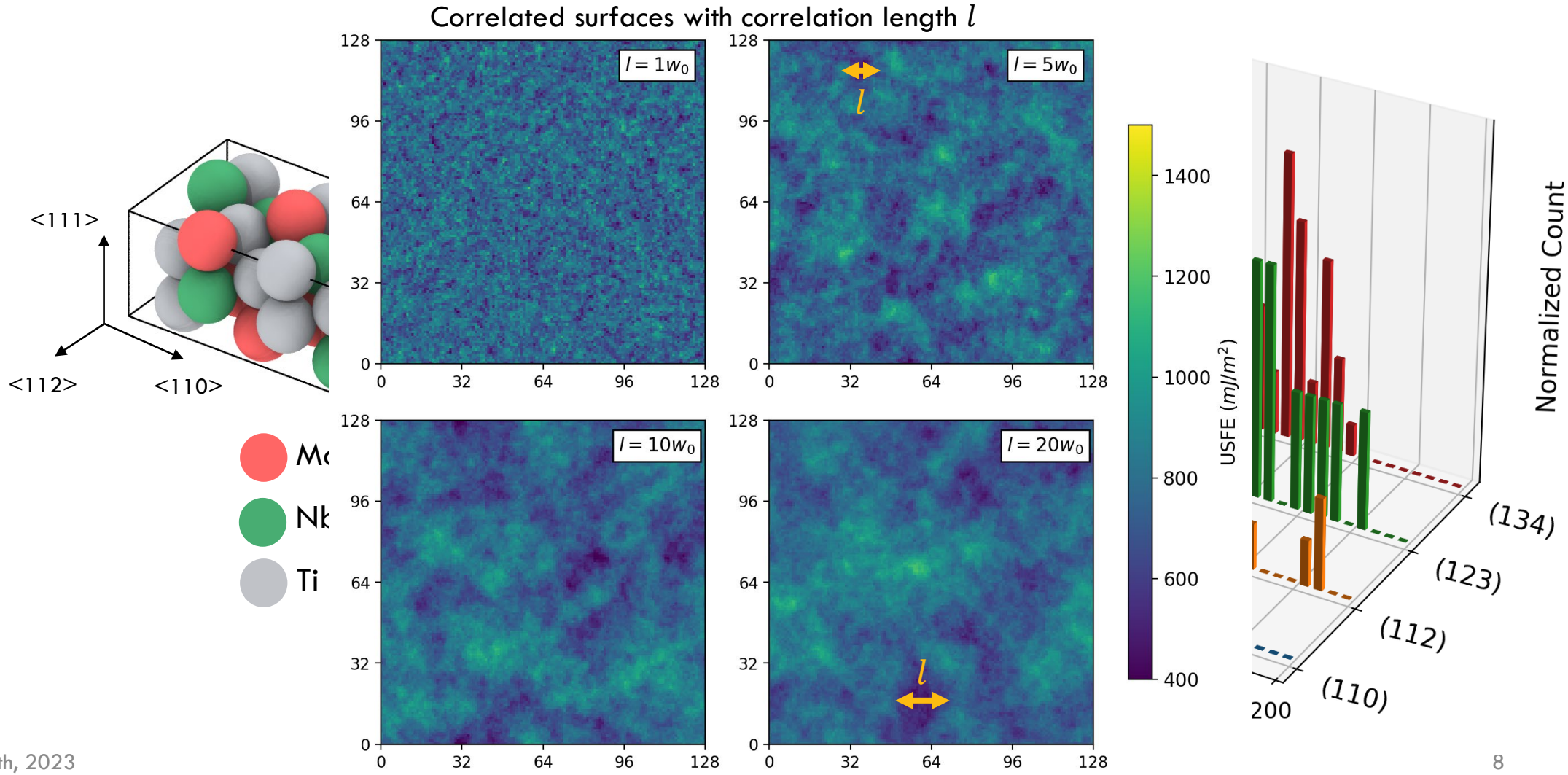
Correlated surfaces with correlation length l

Special quasi-random structure



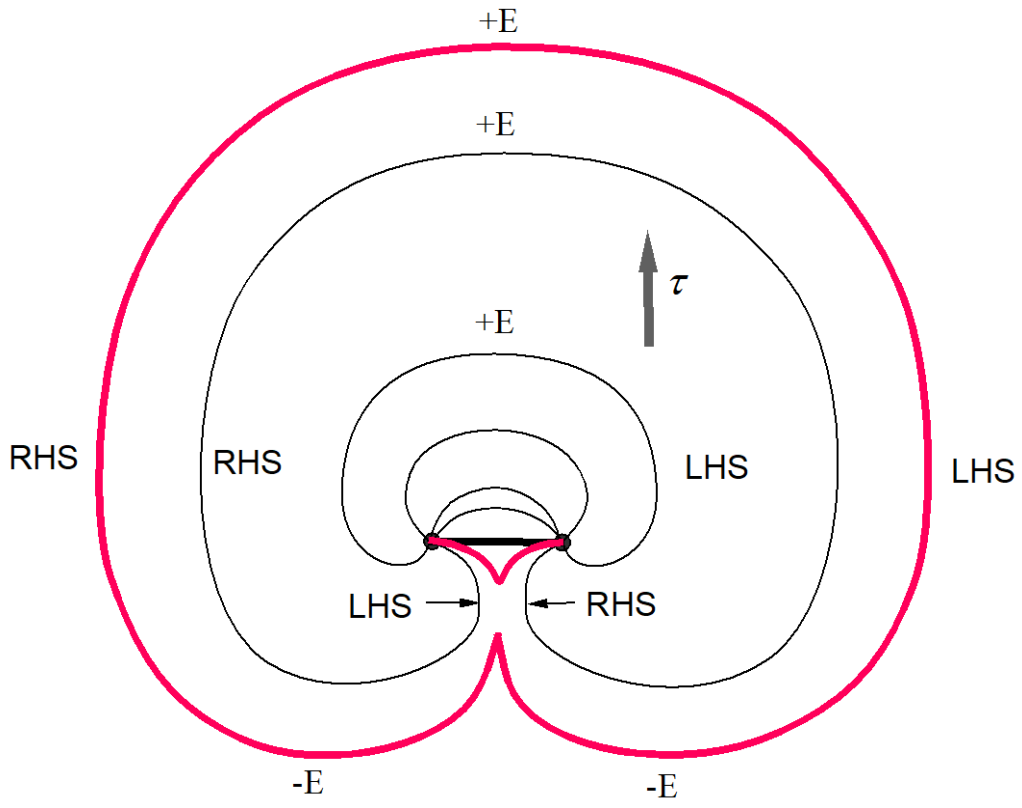


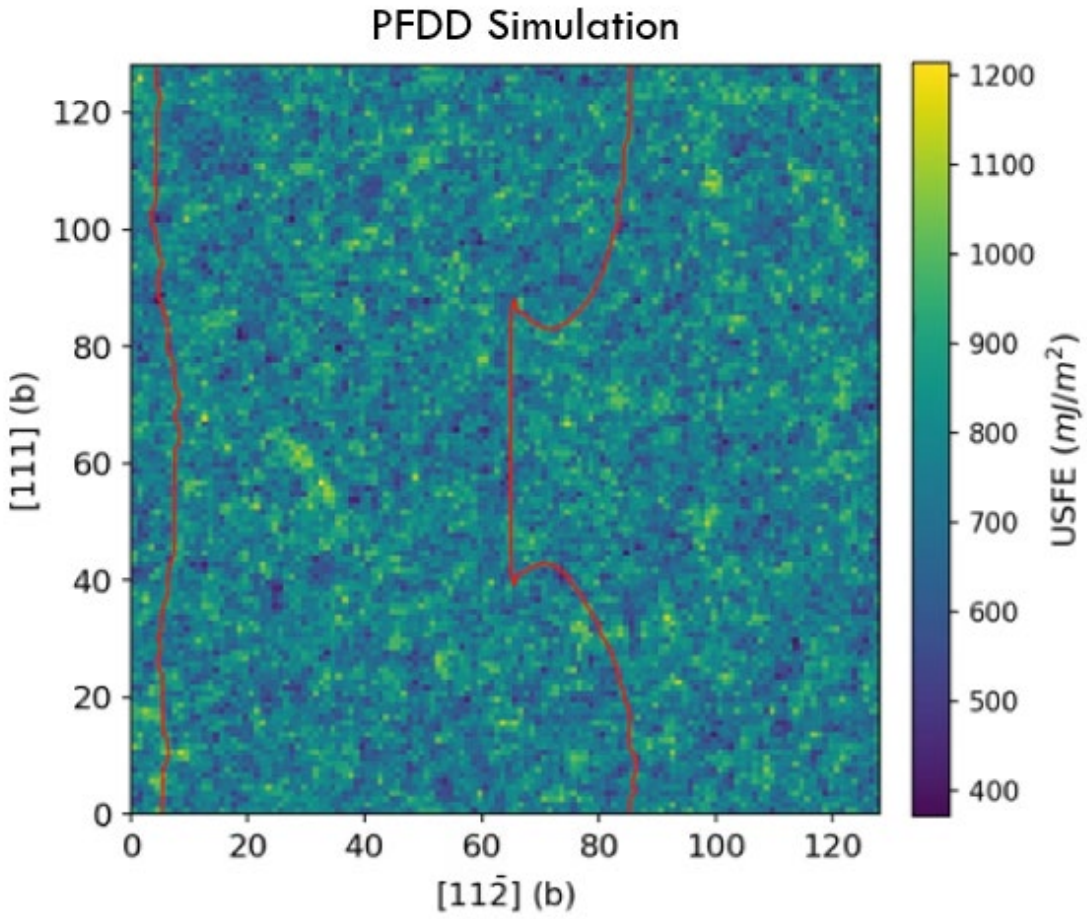
Unstable stacking fault energy – MoNbTi



Simulating dislocation multiplication

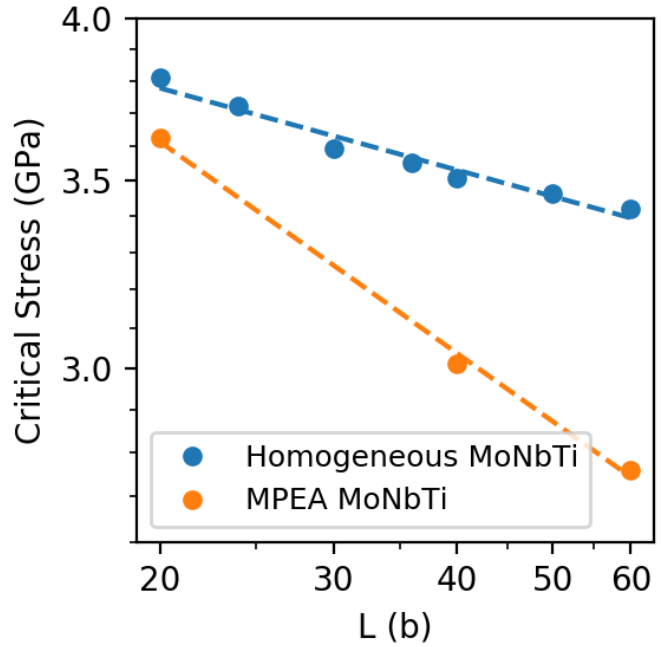
Frank-Read sources are common mechanism for dislocation generation

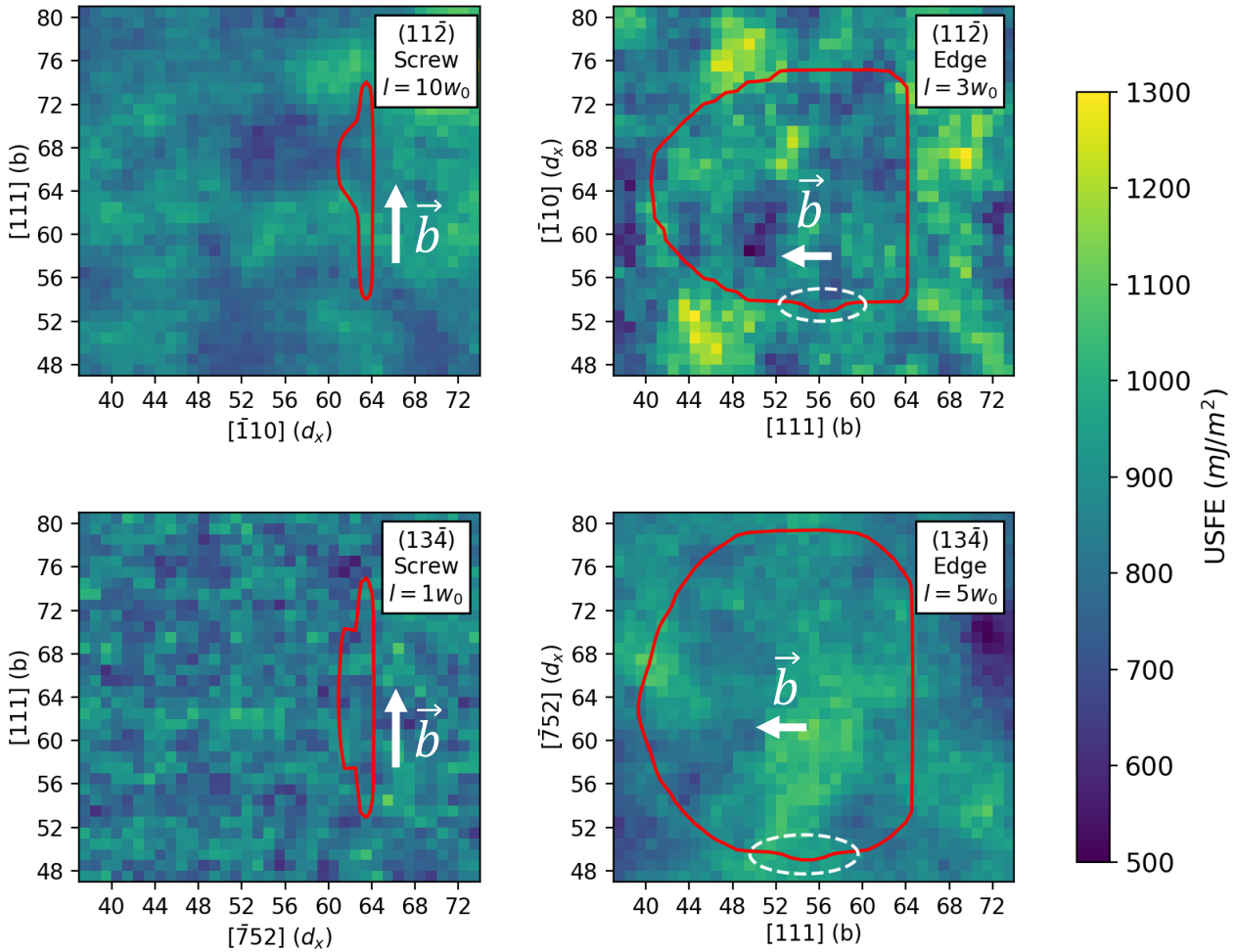




Frank-Read source activation mechanism

- Both screw and edge sources are controlled by kink-pair nucleation into low USFE regions
- Change in mechanism causes more severe scaling with Frank-Read source length



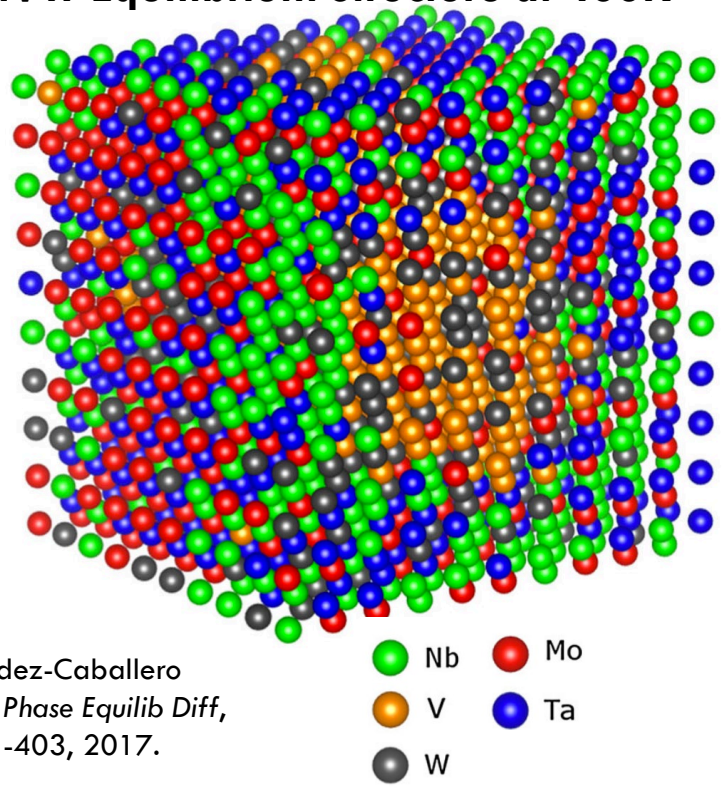


Smith, L. T. W, Su, Y., Xu, S., Hunter, A., & Beyerlein, I. J. (2020). *Int J Plasticity, 134*, 102850.

The role of short-range order in MPEAs

MPEA lattices are disordered in the long-range, but there is thermodynamically driven local order

MoNbTaVW Equilibrium Structure at 400K



Fernández-Caballero et al. *J Phase Equilib Diff*, 38:391-403, 2017.

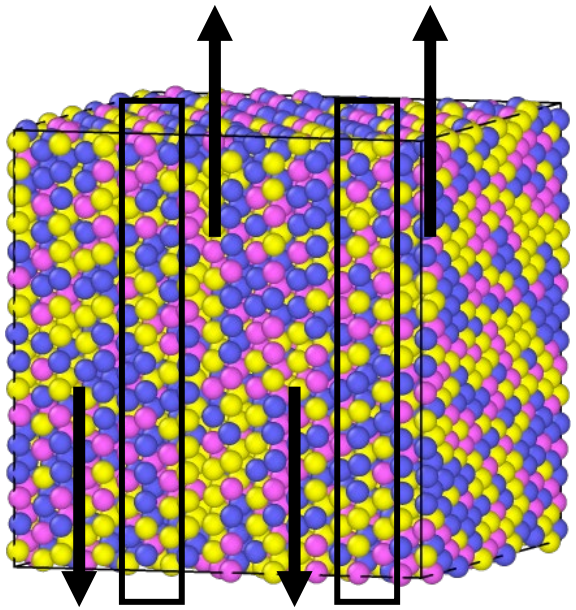
TaNbTi

- Less SRO

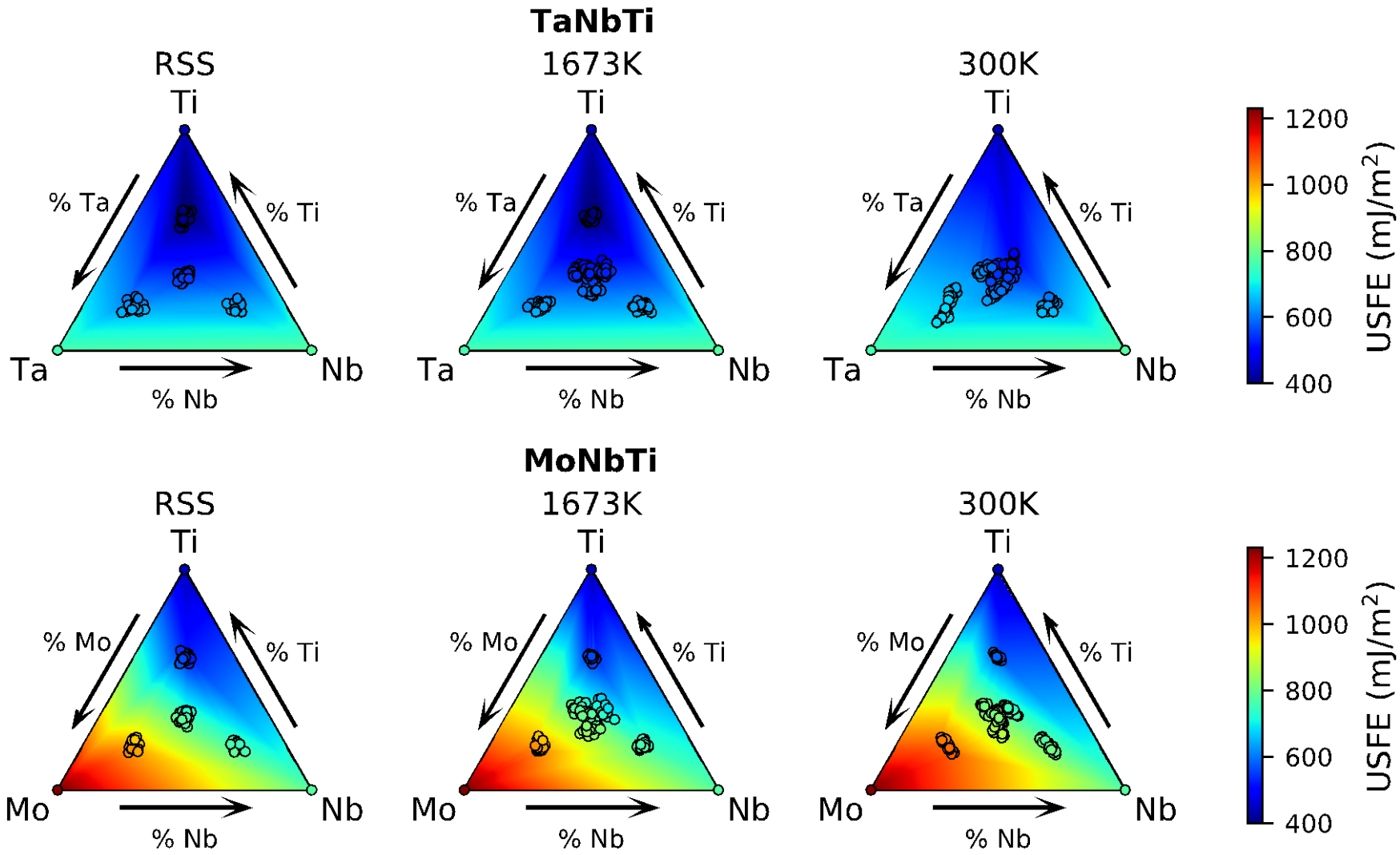
MoNbTi

- More SRO

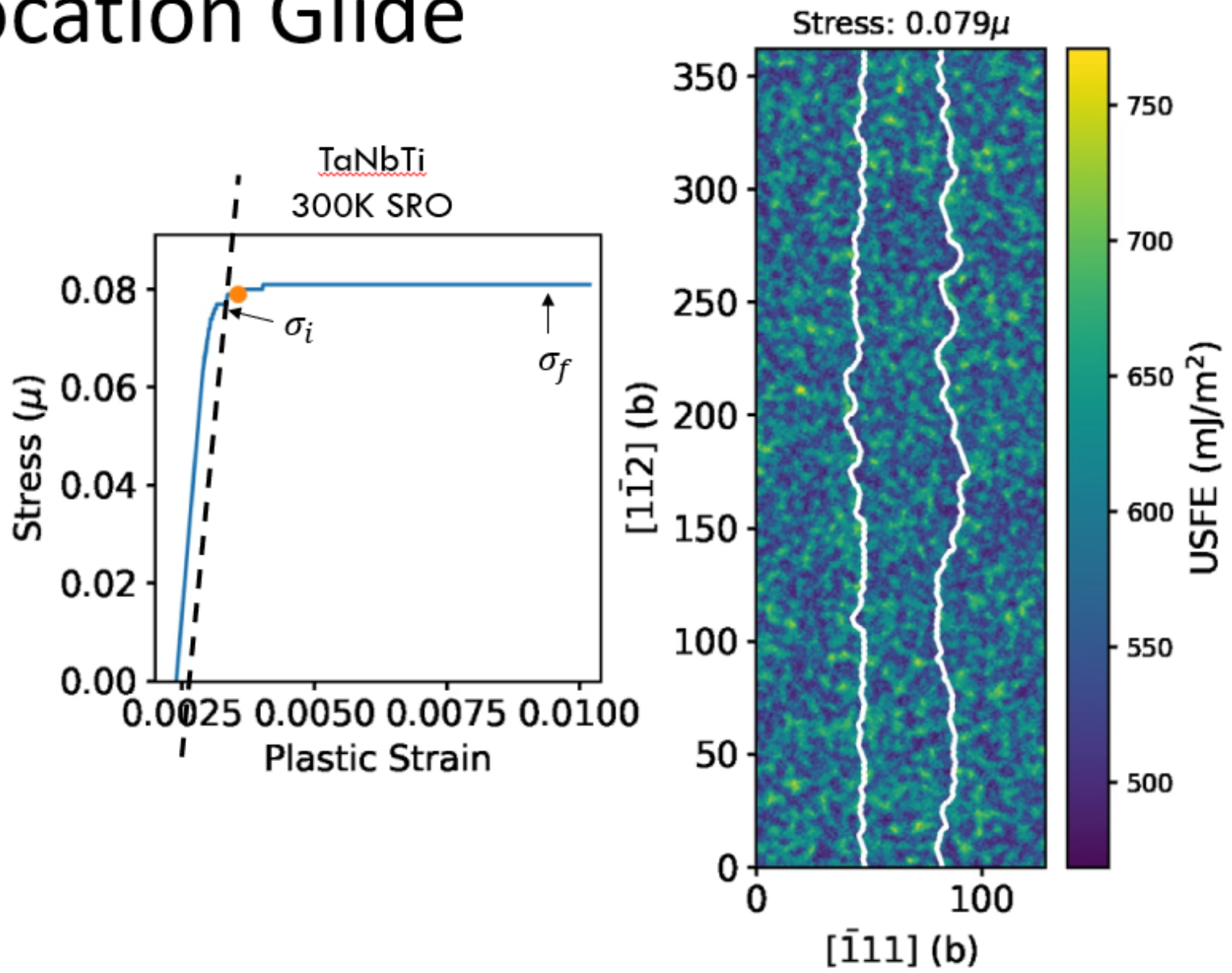
Composition-dependent USFE



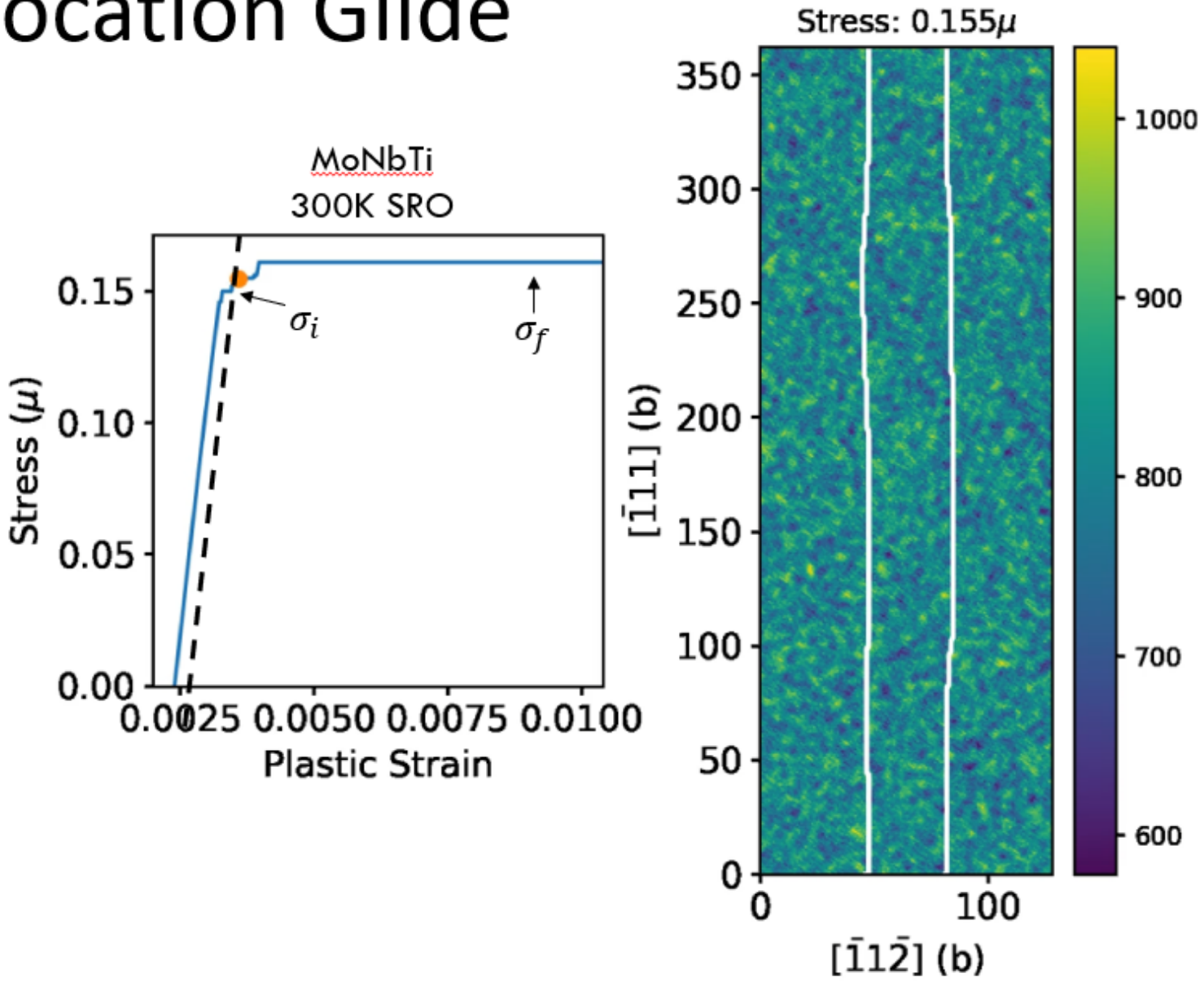
USFE calculated with interatomic potential along different (110) planes with varying local compositions



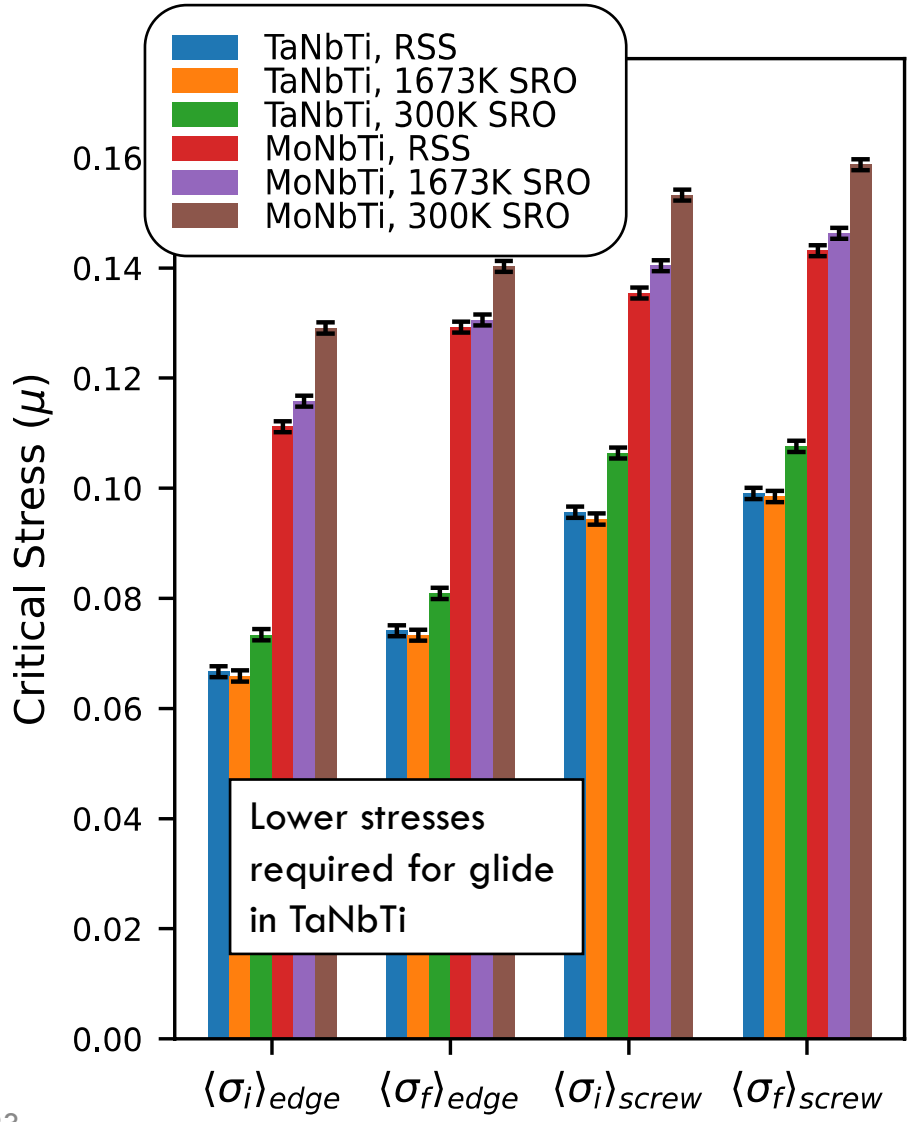
Edge Dislocation Glide

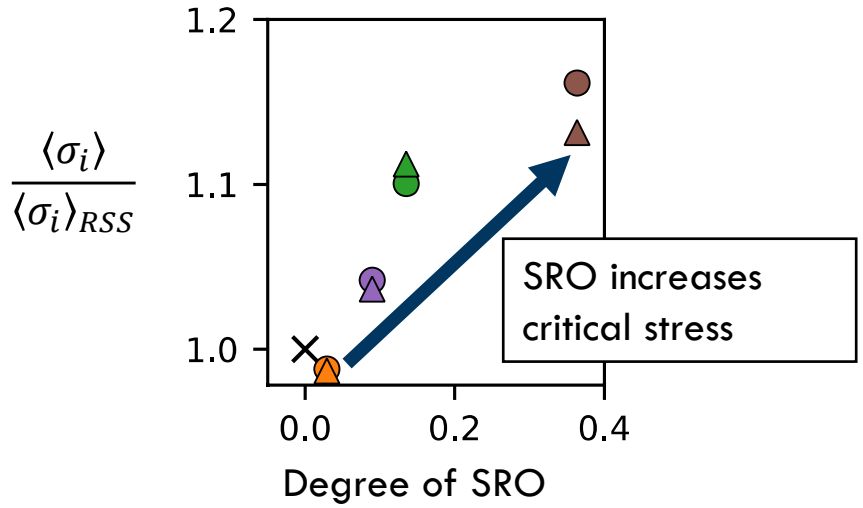


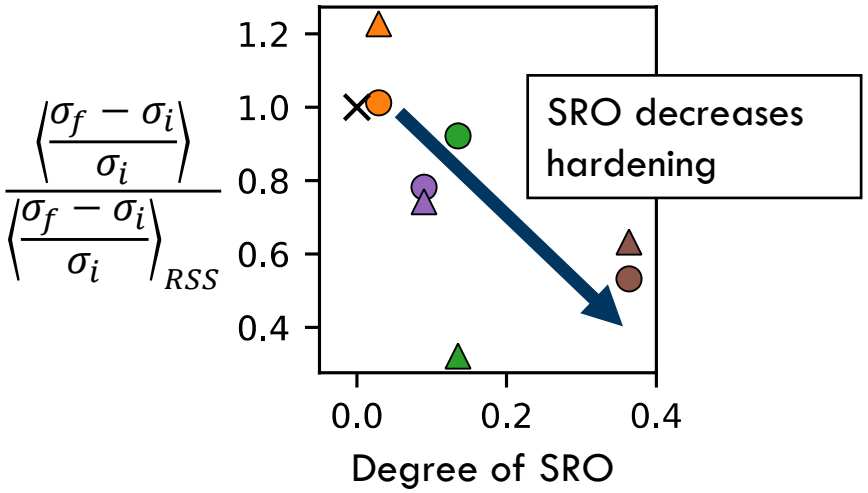
Screw Dislocation Glide



SRO effects on dislocation critical stress







This talk

Part I: Refractory Multi-Principal Element Alloys

Part II: Interstitial Elements in Refractory Alloys

Problem: Interstitial Embrittlement

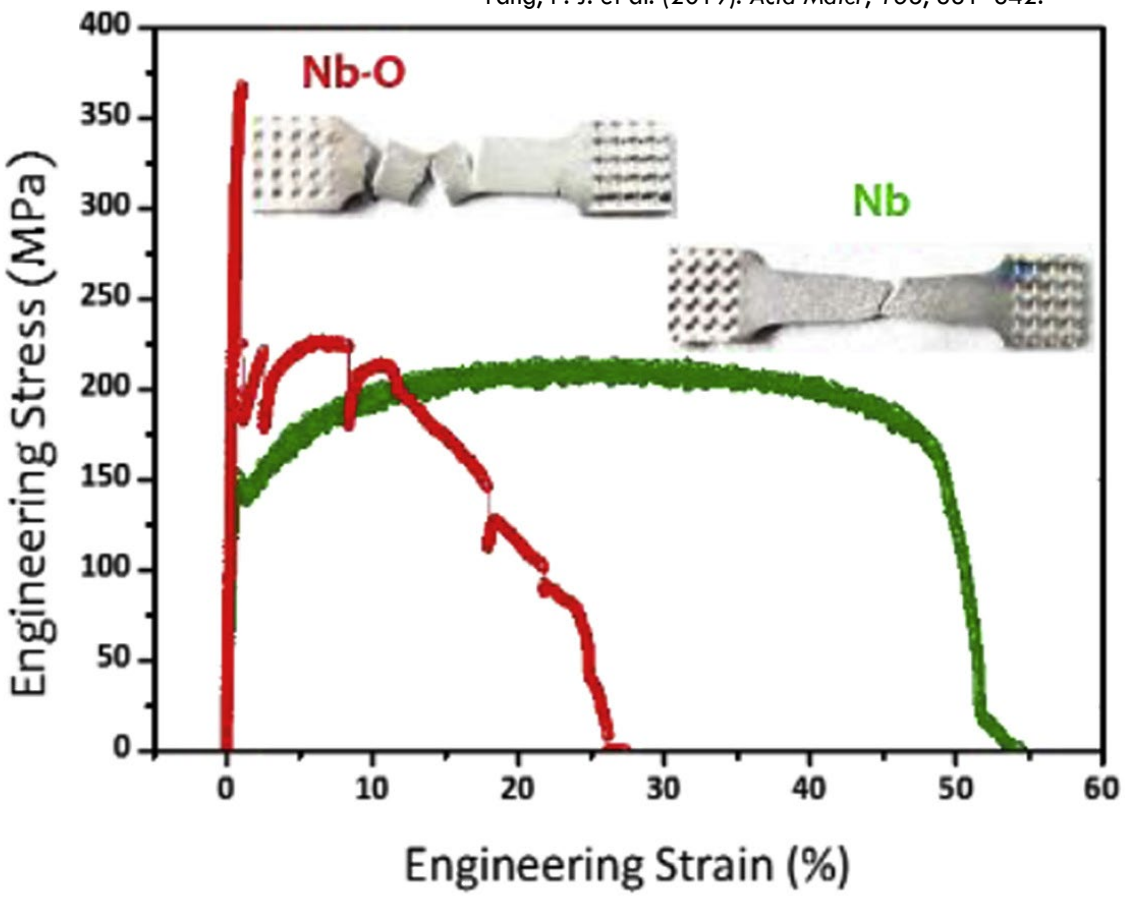
- Refractory metals easily absorb interstitial contaminants like O, H, and C from the atmosphere

- Interstitials generally increase yield strength at the expense of ductility

How do interstitials affect dislocation mechanisms and stresses?

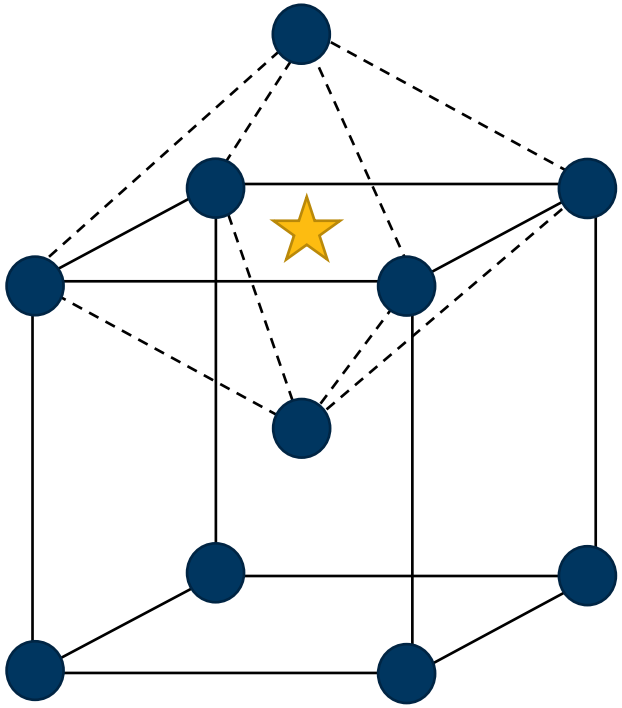
Model systems: Nb-O and W-H

Yang, P. J. et al. (2019). *Acta Mater*, *168*, 331–342.

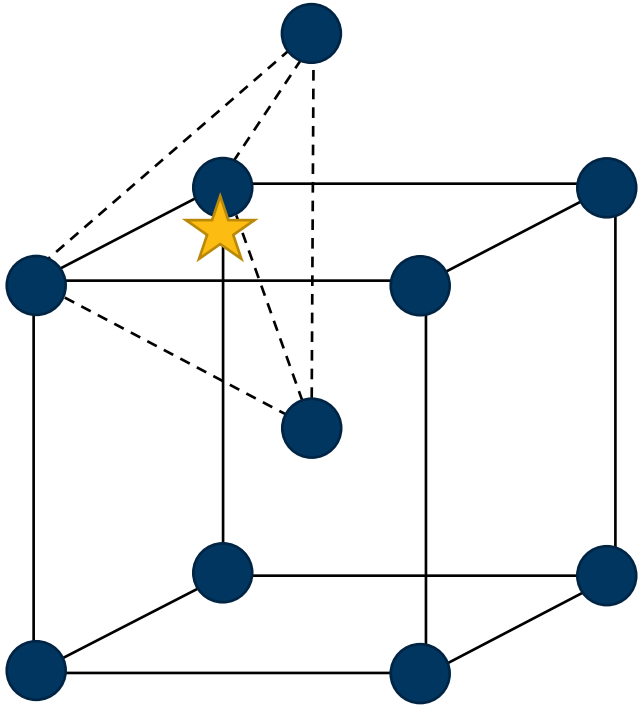


Interstitials in BCC lattices

- Interstitials create a distortion in the lattice
- Interstitials can interact with dislocations via their stress fields (long-range) or directly at the dislocation core (short-range)



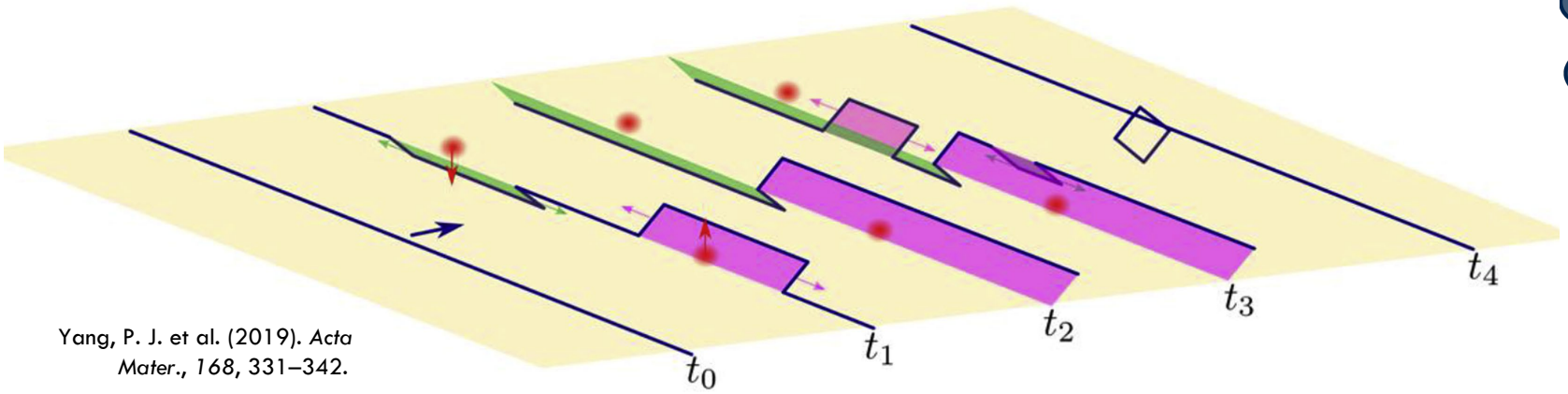
Octahedral site



Tetrahedral site

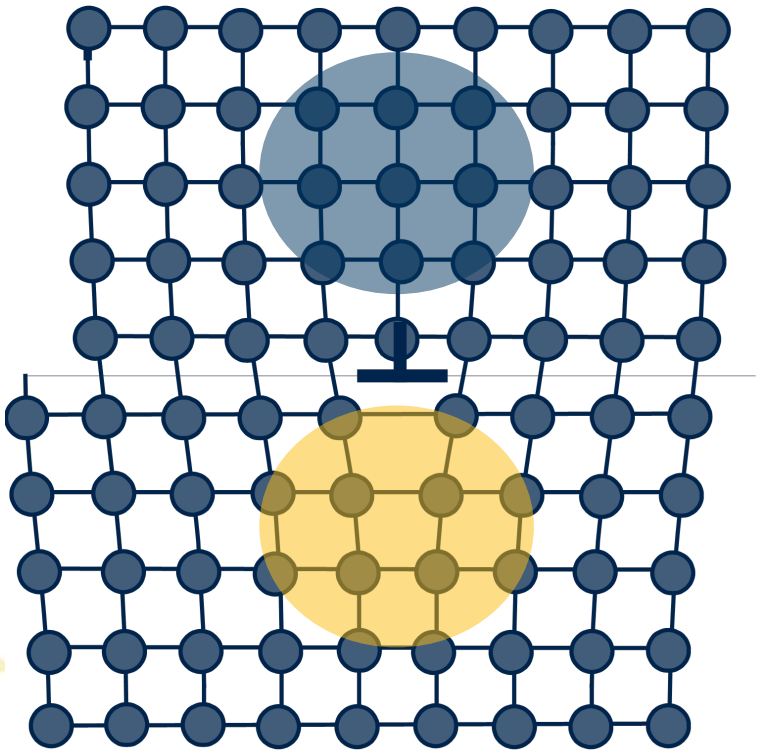
Long-Range Interactions

- Dislocations have long-range stress fields: $\sigma \propto \frac{1}{r}$
- Interstitials interact with these stress fields and form atmospheres around dislocation cores
- Interstitials can pin dislocations or cause cross slip and debris formation



Yang, P. J. et al. (2019). *Acta Mater., 168*, 331–342.

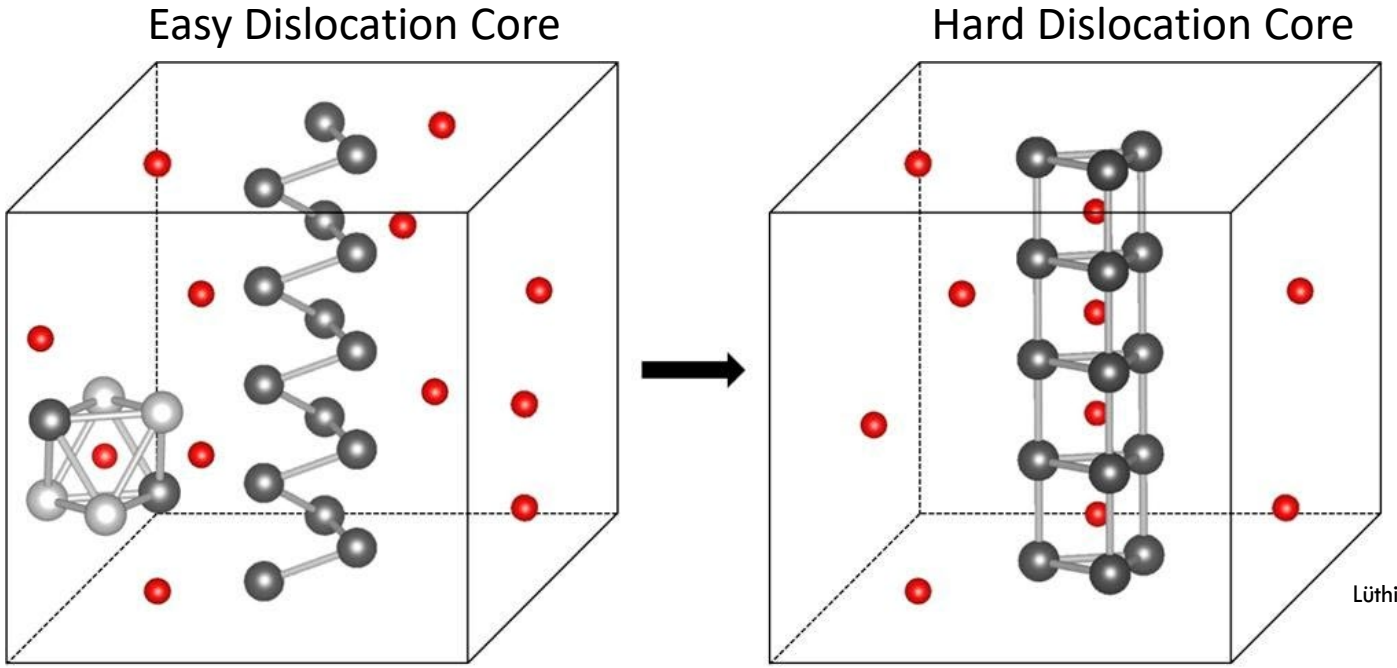
Edge Dislocation



Cai, W., & Nix, W. D. (2016). *Imperfections in Crystalline Solids.*

Short-Range Interactions

- Interstitials change the structure and energy of a dislocation core
- Binding energy at dislocation core can pin the dislocation



Lüthi, B. et al. (2018). *Computational Materials Science, 148*, 21–26.

Interstitials in PFDD

- PFDD tracks dislocation structure through ϕ
  - $\phi = 0$: Unslipped
  - $\phi = 1$: Slipped
  - $0 < \phi < 1$: Dislocation

$$E = E_{elas} + E_{ext} + E_{lattice}$$

Elastic interaction energy

$$E_{elas}(\phi) = \frac{1}{2}[\epsilon - \epsilon^p(\phi)] \cdot C[\epsilon - \epsilon^p(\phi)]$$

Externally applied energy

$$E_{ext}(\phi) = \sigma^{app} \cdot \epsilon^p(\phi)$$

Energy to break bonds (material specific)

$$E_{lattice}(\phi) = \frac{E_{USFE}}{d_{slip}} \sin^2 \pi\phi$$

Interstitials in PFDD

- PFDD tracks dislocation structure through ϕ
  - $\phi = 0$: Unslipped
  - $\phi = 1$: Slipped
  - $0 < \phi < 1$: Dislocation
- Add a new parameter c to track local interstitial concentration

$$E = E_{elas} + E_{ext} + E_{lattice}$$

Elastic interaction energy

$$E_{elas}(\phi, c) = \frac{1}{2}\left[\epsilon - \epsilon^{p}(\phi) - \epsilon^{int}(c)\right] \cdot C\left[\epsilon - \epsilon^{p}(\phi) - \epsilon^{int}(c)\right]$$

Long-range, elastic interactions

Externally applied energy

$$E_{ext}(\phi) = \sigma^{app} \cdot \epsilon^{p}(\phi)$$

Energy to break bonds (material specific)

$$E_{lattice}(\phi, c) = \frac{E_{USFE}(c)}{d_{slip}} \sin^2 \pi\phi$$

Short-range, core interactions

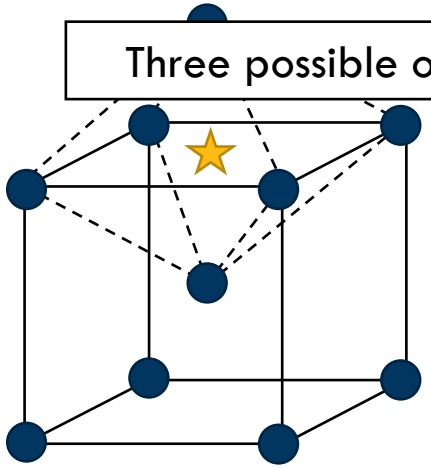
Long-range interactions in PFDD

$$E_{elas}(\phi, c) = \frac{1}{2}\left[\epsilon - \epsilon^{p}(\phi) - \epsilon^{int}(c)\right] \cdot C\left[\epsilon - \epsilon^{p}(\phi) - \epsilon^{int}(c)\right]$$

- Interstitial strain given by $\epsilon^{int}(c) = \lambda^{int} c$
  - λ^{int} determined from experiments or atomistic calculations

Nb-O

Three possible orientations

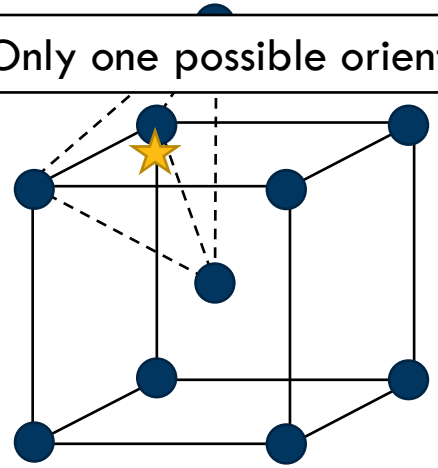


$$\lambda^{int} = \begin{pmatrix} 0.485 & 0 & 0 \\ 0 & -0.0645 & 0 \\ 0 & 0 & -0.0645 \end{pmatrix}$$

O occupies octahedral sites

W-H

Only one possible orientation



$$\lambda^{int} = \begin{pmatrix} 0.0677 & 0 & 0 \\ 0 & 0.0677 & 0 \\ 0 & 0 & 0.0677 \end{pmatrix}$$

H occupies tetrahedral sites

Short-range interactions in PFDD

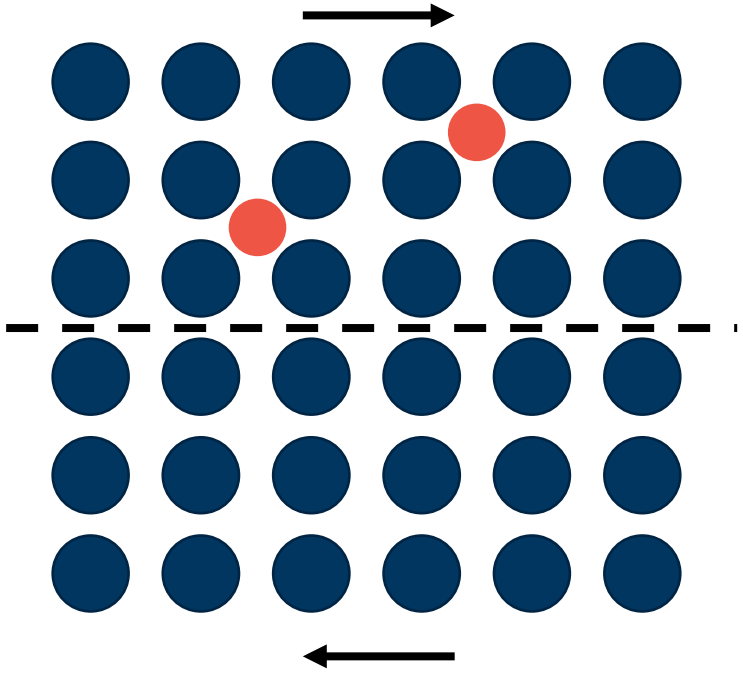
$$E_{lattice}(\phi, c) = \frac{E_{USFE}(c)}{d_{slip}} \sin^2 \pi\phi$$

- Need to calculate USFE for different interstitial concentrations
- Idea: calculate interaction energy of different interstitial sites
  - E_{int-SF}: change in stacking fault energy due to interstitial

$$E_{USFE}(c) = E_{USFE}(0) + \sum \frac{c^i E^i_{int-SF}}{A}$$

Pure metal USFE

Adjustment due to interstitials



Evolution of concentration in PFDD

Dislocation slip is **non-conserved**:

$$\frac{d\phi}{dt} = -m_{disl}\frac{\partial E}{\partial \phi}$$

Interstitial concentration is **conserved**:

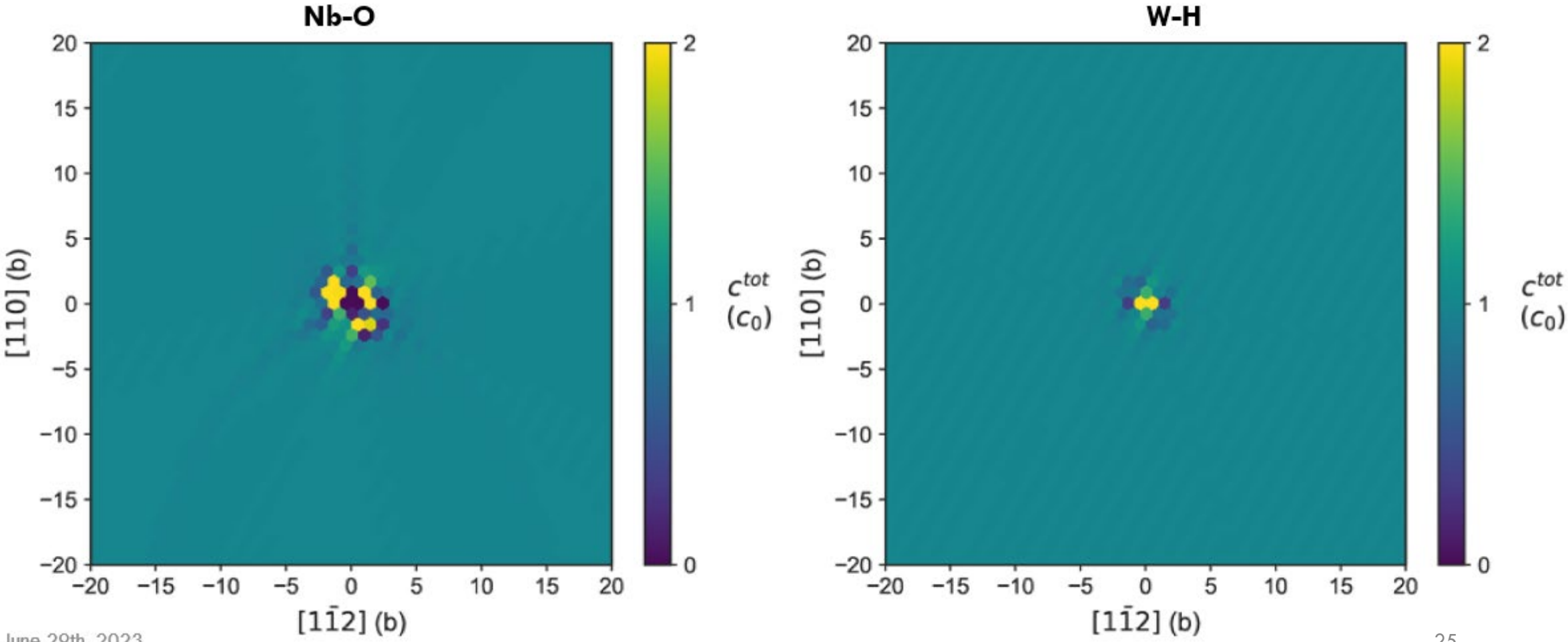
$$\frac{dc}{dt} = \nabla \cdot (m_{int}\nabla \mu)$$

Chemical potential: $\mu = \frac{\partial E}{\partial c}$

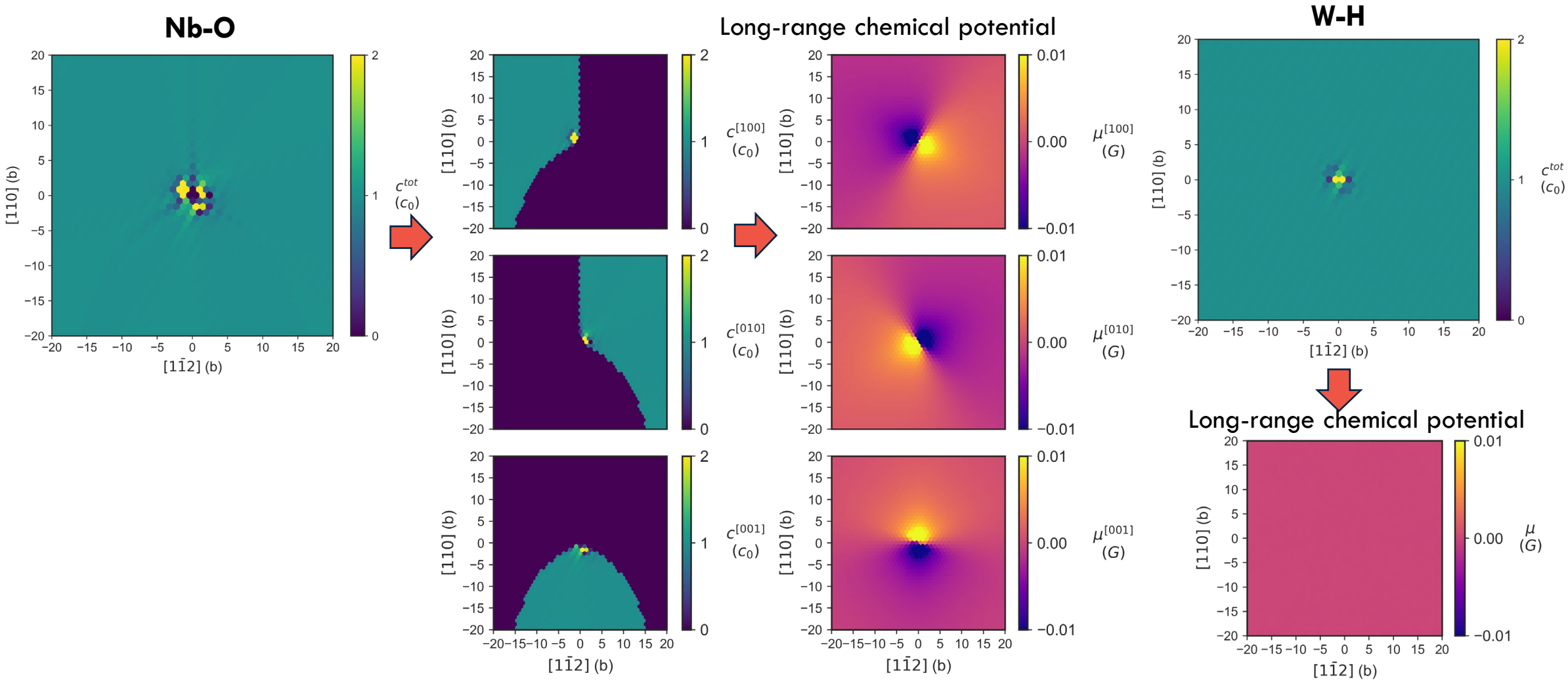
- Interstitials will flow towards lower chemical potential regions
- When there are multiple site types/orientations available, interstitials adopt the lowest energy configuration

Screw dislocation interstitial atmospheres

Initially homogeneous concentration c_0 = 0.01

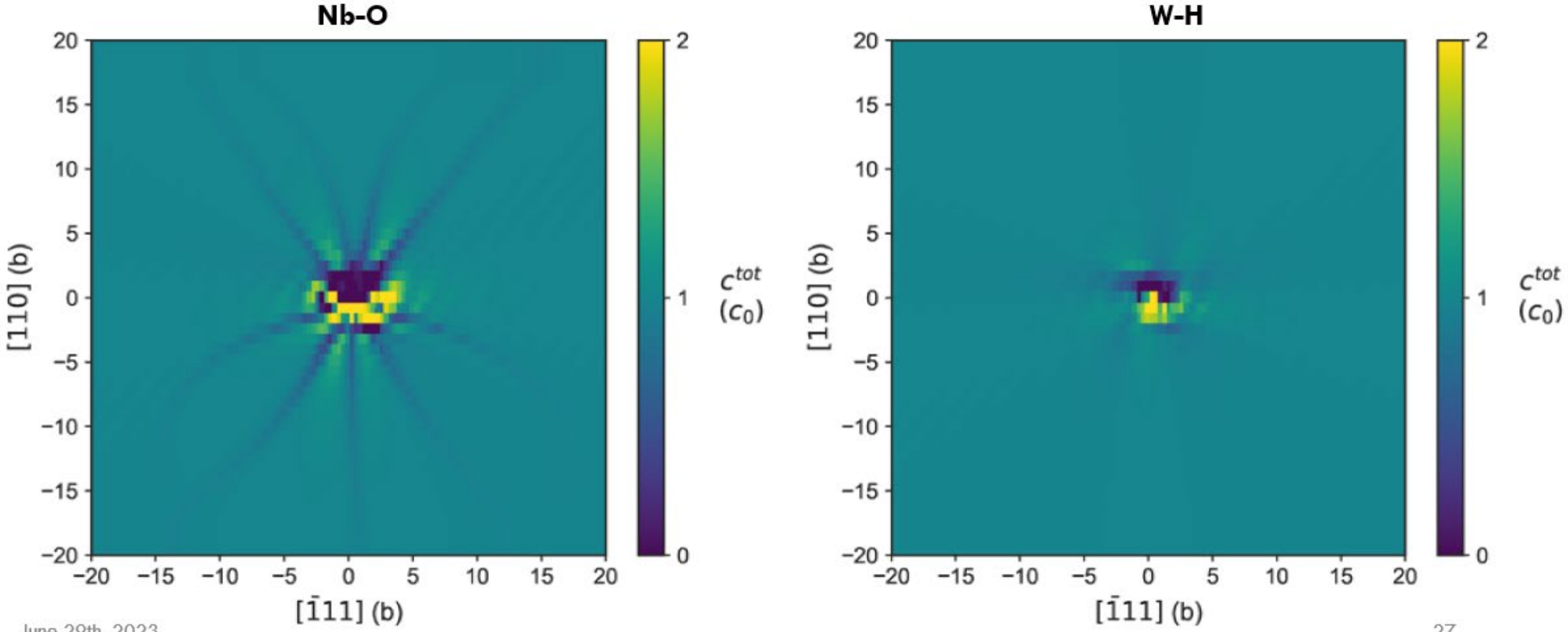


Screw dislocation interstitial atmospheres



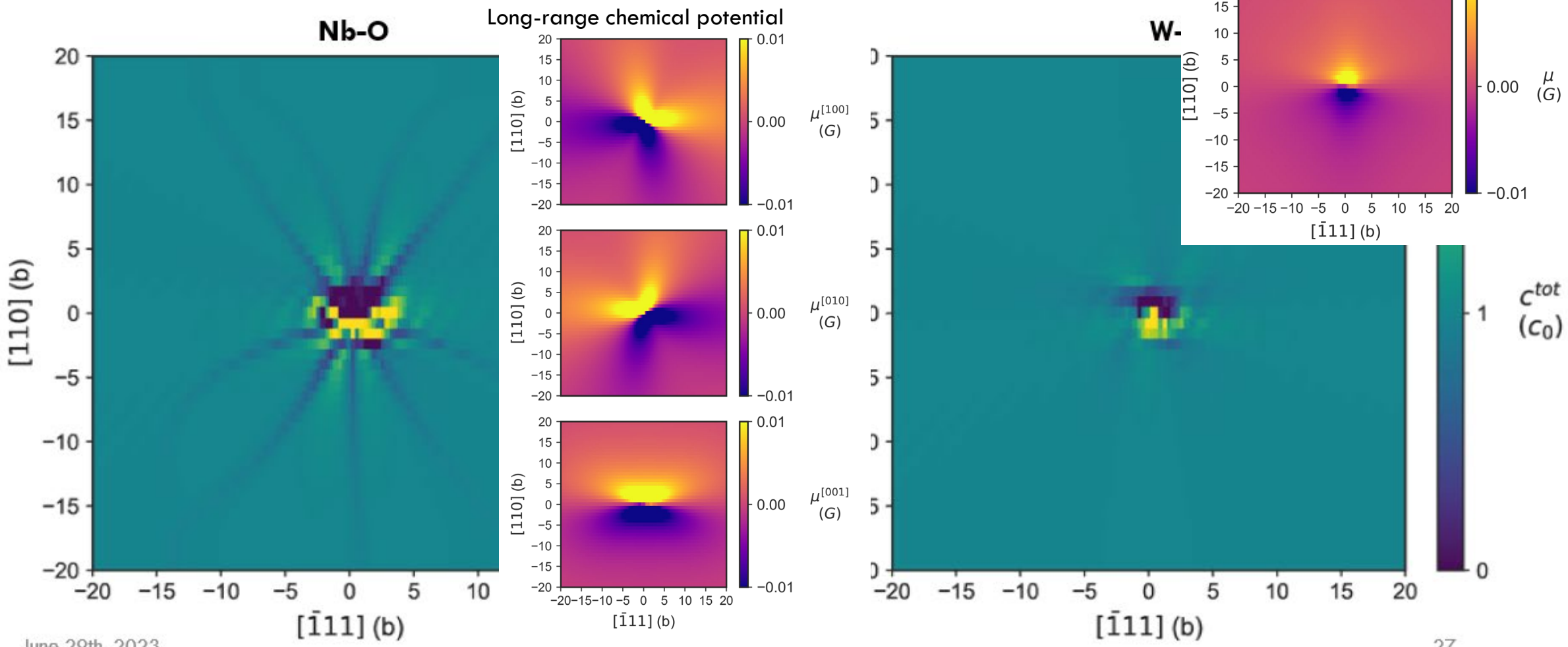
Edge dislocation interstitial atmospheres

Initially homogeneous concentration c_0 = 0.01



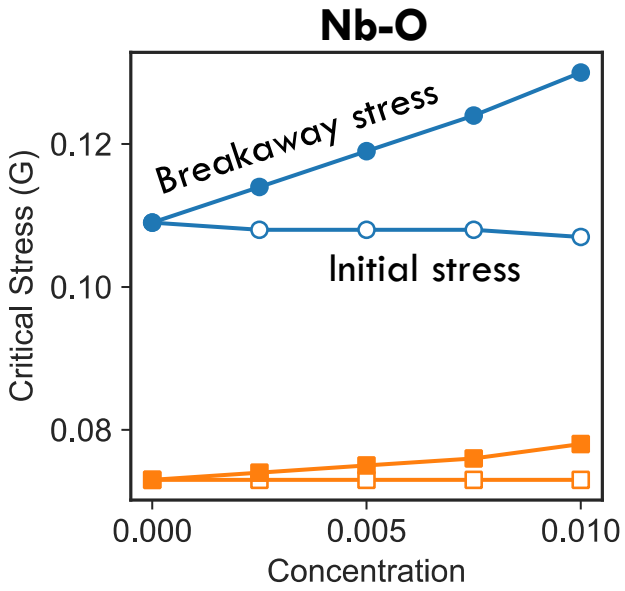
Edge dislocation interstitial atmospheres

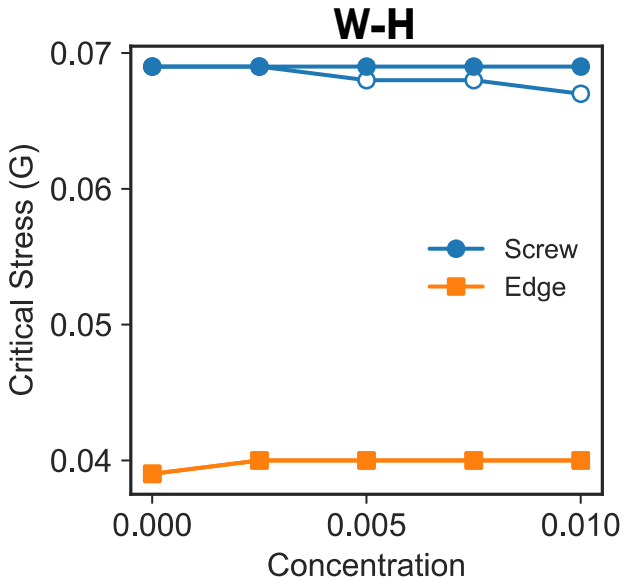
Initially homogeneous concentration c_0 = 0.01



Critical glide stresses

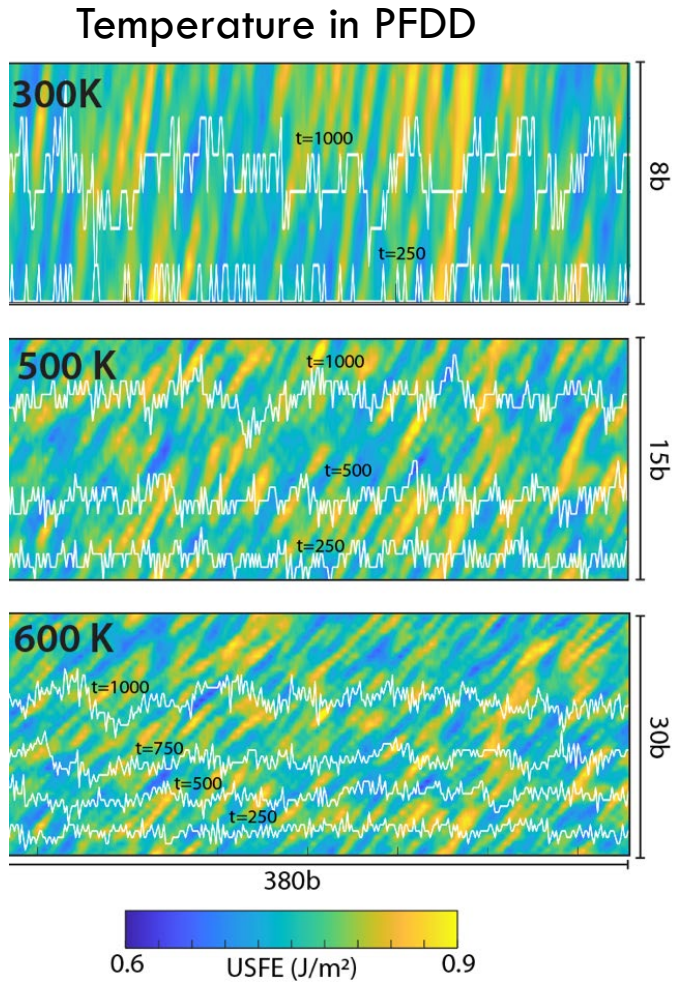
- Dislocations can glide a short distance before becoming pinned again (initial stress)
- Screw dislocation initial stress decreases with interstitial concentration for both Nb-O and W-H
- Breakaway stress for Nb-O increases with O concentration
- Breakaway stress for W-H is largely unaffected by concentration for both screw and edge





Conclusions and Outlook

- Refractory MPEAs show promise as high-temperature materials
  - Dislocation mechanisms in MPEAs differ from pure refractory alloys
  - Dislocations controlled by athermal kink-pair nucleation
  - SRO increases critical dislocation stresses
- Interstitial-dislocation interactions must be understood for refractory alloys
  - O and H create different atmospheres due to their different site type occupation
  - H and O can alter dislocation behavior in opposite ways
- Future work
  - Include temperature in PFDD for thermally-activated mechanisms (kink-pair nucleation)



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Thank you!

Temperature in PFDD