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# Multiscale modelling of plasticity in BCC metals from ab initio methods

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Y. Zhao<sup>1,4</sup>, J. Marian.<sup>4</sup>

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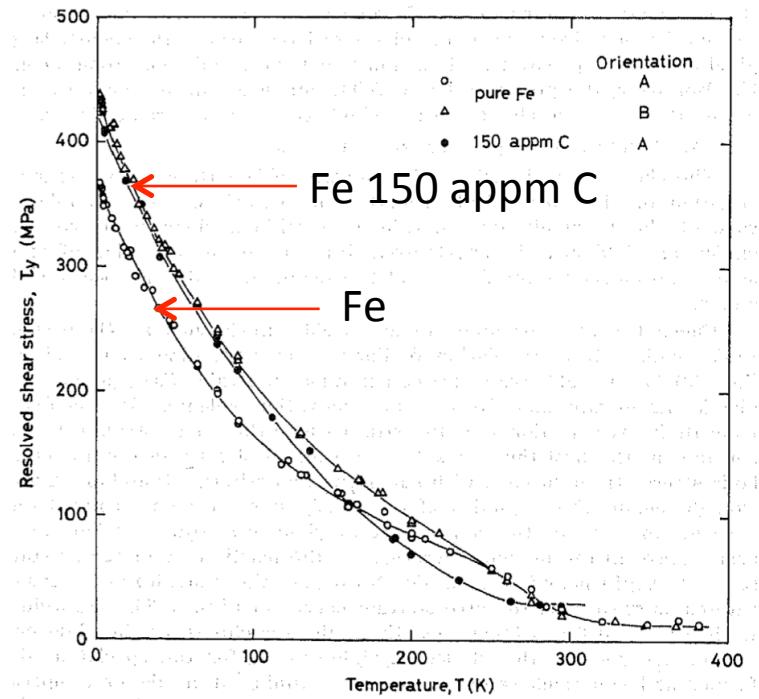
LabEx Meeting WP4 – WP5

February, 27<sup>th</sup> 2019



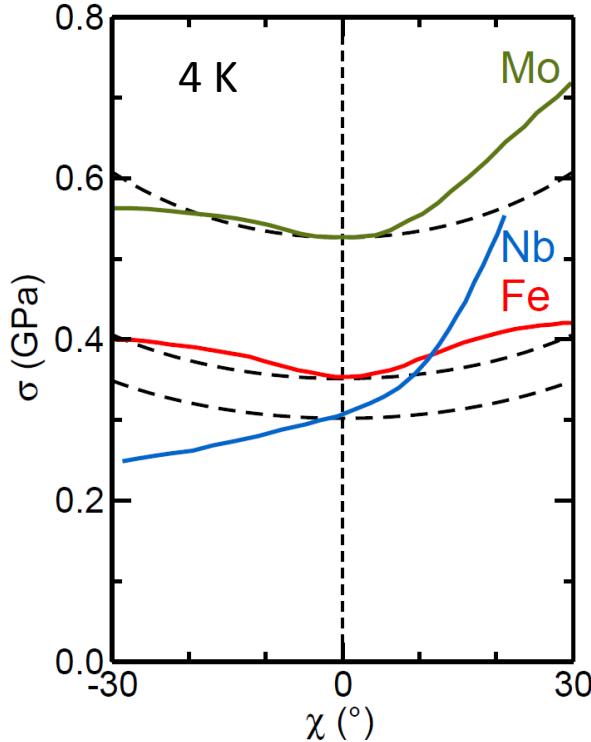
# Motivations

Aono et al. (1981)



- CRSS depends on temperature and interstitial concentration

Aono et al. (1984)

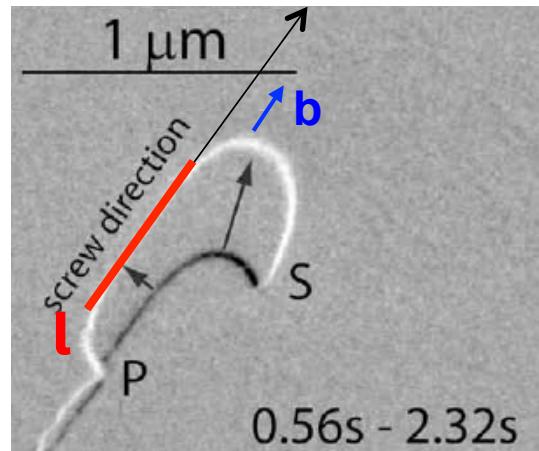


- Schmid law deviation
- metal-dependent

Need for macroscopic models adapted to BCCs

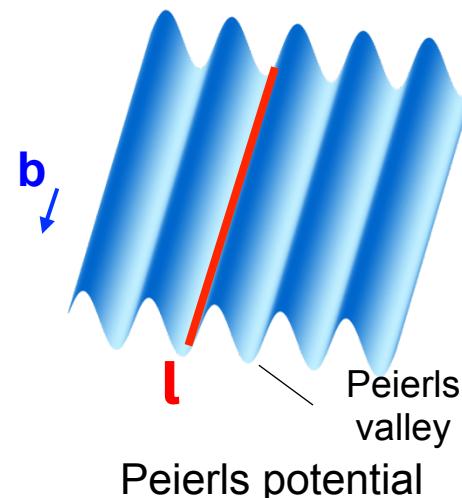
# Multiscale plasticity of BCC metals

## Microscopic

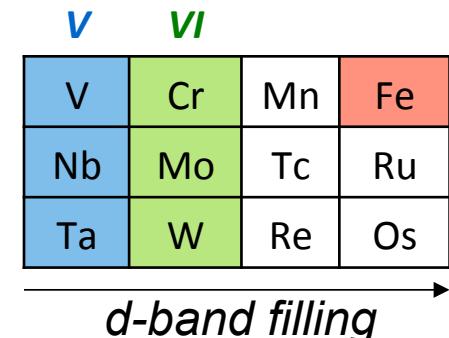


TEM screw dislocation pure Fe  
Caillard, Acta Mater. **58**, 3493 (2010)

## Atomic



## Electronic



Low mobility of  
 $\frac{1}{2} <111>$  screw  
dislocations

Strong core effects  
Deep Peierls valleys

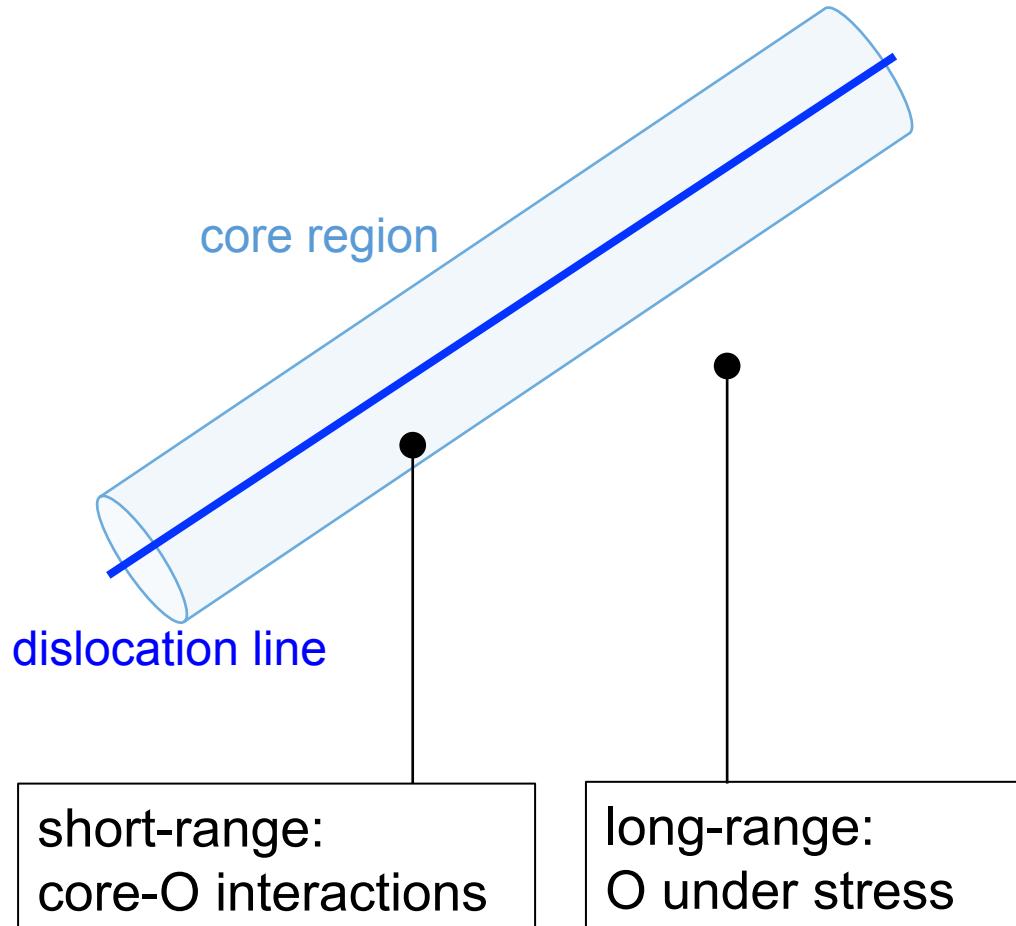
Need for ab initio  
simulations

Need for ab initio input

# Outline

1. Dislocation-O coevolution in W
  - a. Ab initio investigation
  - b. upscaling with kMC
2. Schmid law deviation in BCCs
3. Ab initio modelling of dislocations cores in FCC metals  
*LabEx project for 2019-2020*

# Dislocation-O interactions in W



Calculated with ab initio:

- O stability in W
- O migration under strain

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{bmatrix}$$

hydrostatic

$$\boldsymbol{\varepsilon} = \begin{bmatrix} 0 & \gamma/2 & 0 \\ \gamma/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

shear

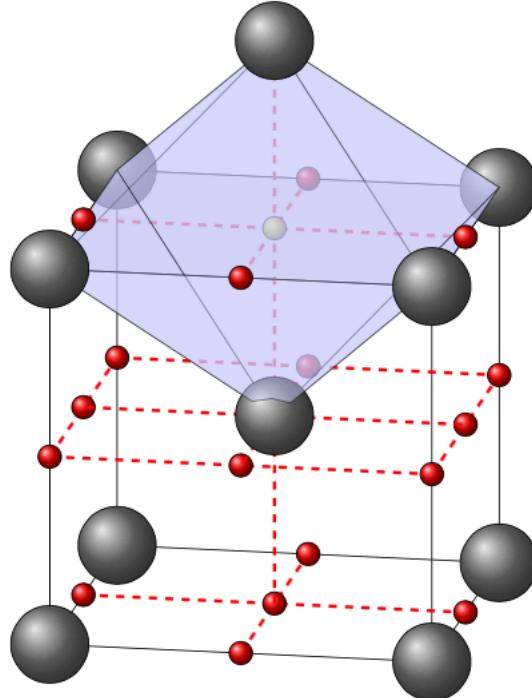
- dislocation core-O interactions

# O stability in W

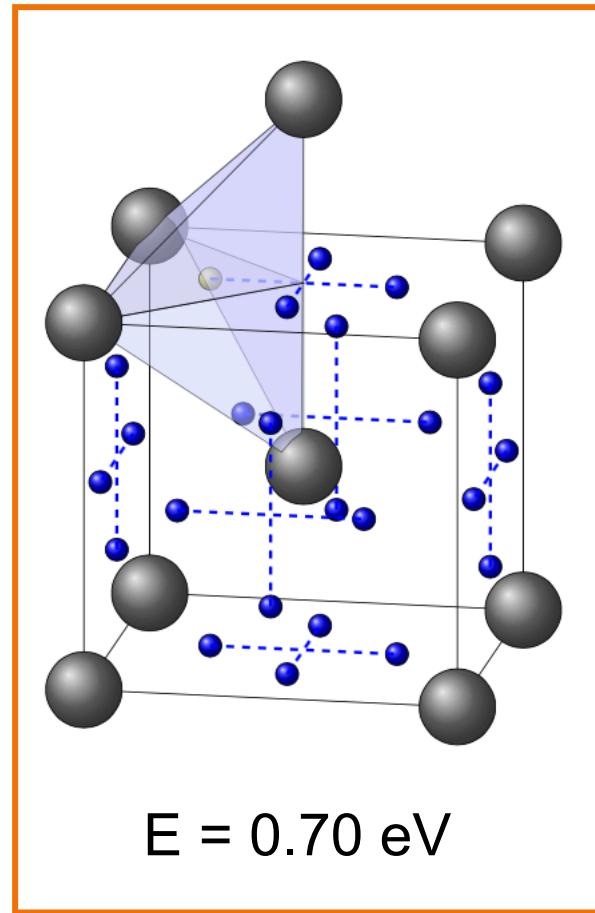
Y. Zhao, L. Dezerald, J. Marian, Metals (2019)



- bcc lattice sites
- octahedral sites
- tetrahedral sites



$$E = 1.01 \text{ eV}$$

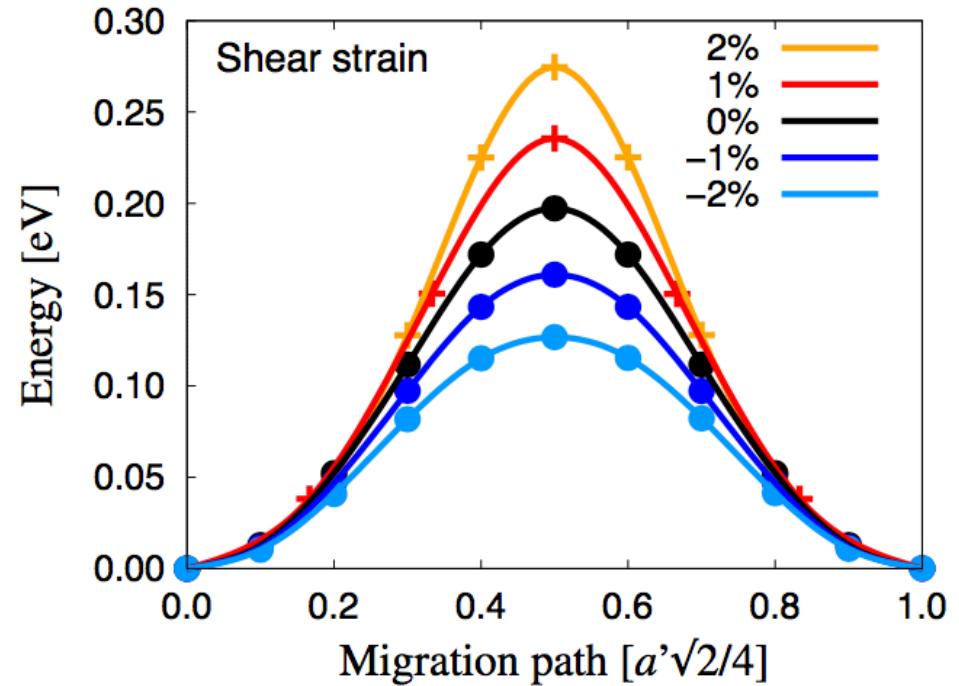
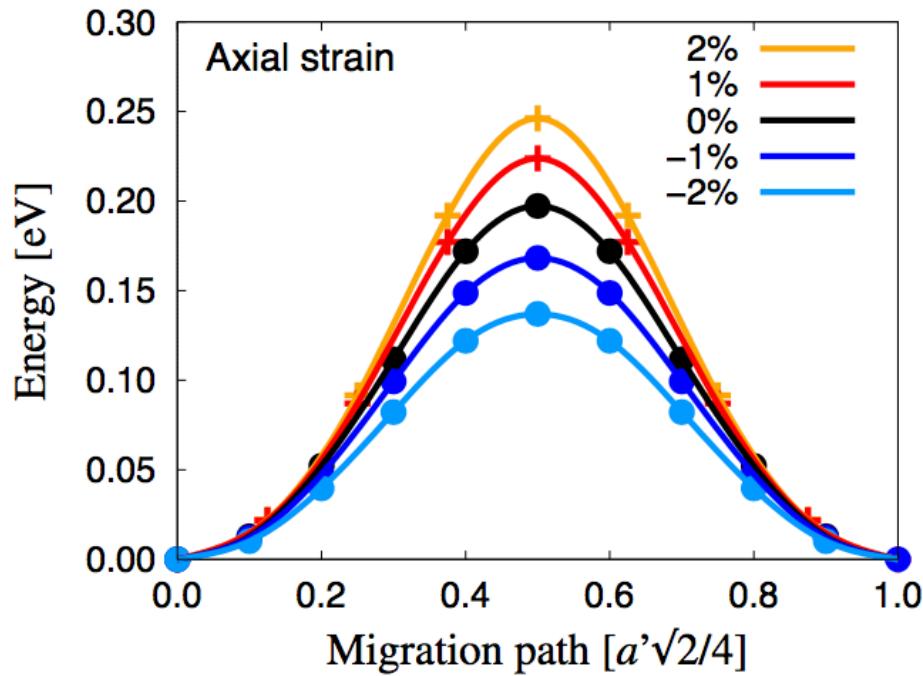


$$E = 0.70 \text{ eV}$$

O stable in Tetrahedral sites

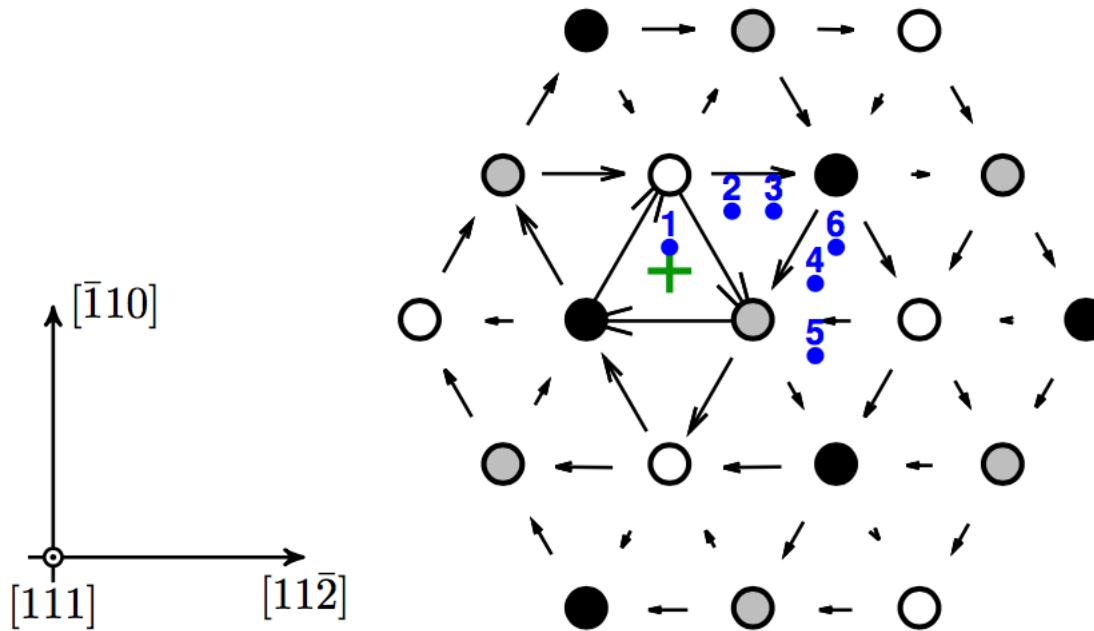
# O migration in bulk W

Y. Zhao, L. Dezerald, J. Marian, Metals (2019)



Long-range dislocation-O interactions with ab initio

# Dislocation core-O interactions

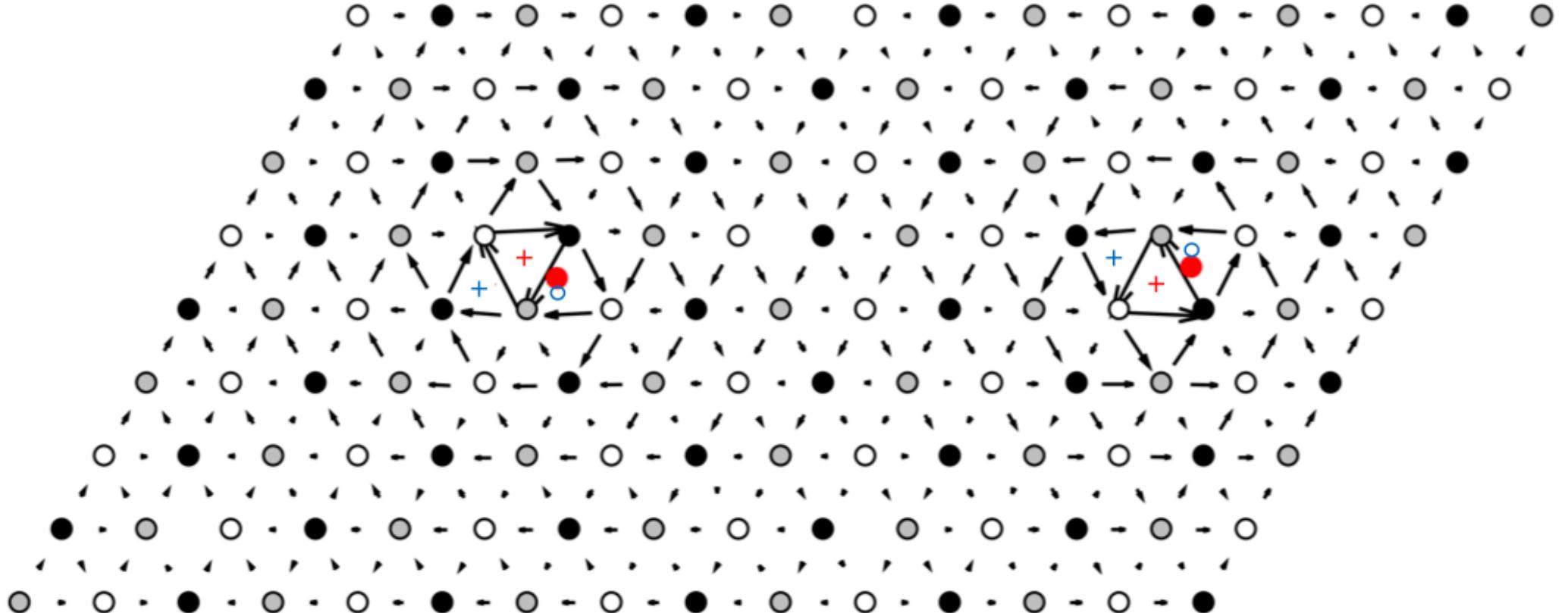


Initial configuration (before relaxation)

- Easy core for dislocation
- W in tetrahedral sites up to 6<sup>th</sup> nearest neighbor from the dislocation center

# Dislocation core-O interactions

Y. Zhao, L. Dezerald, J. Marian, Metals (2019)



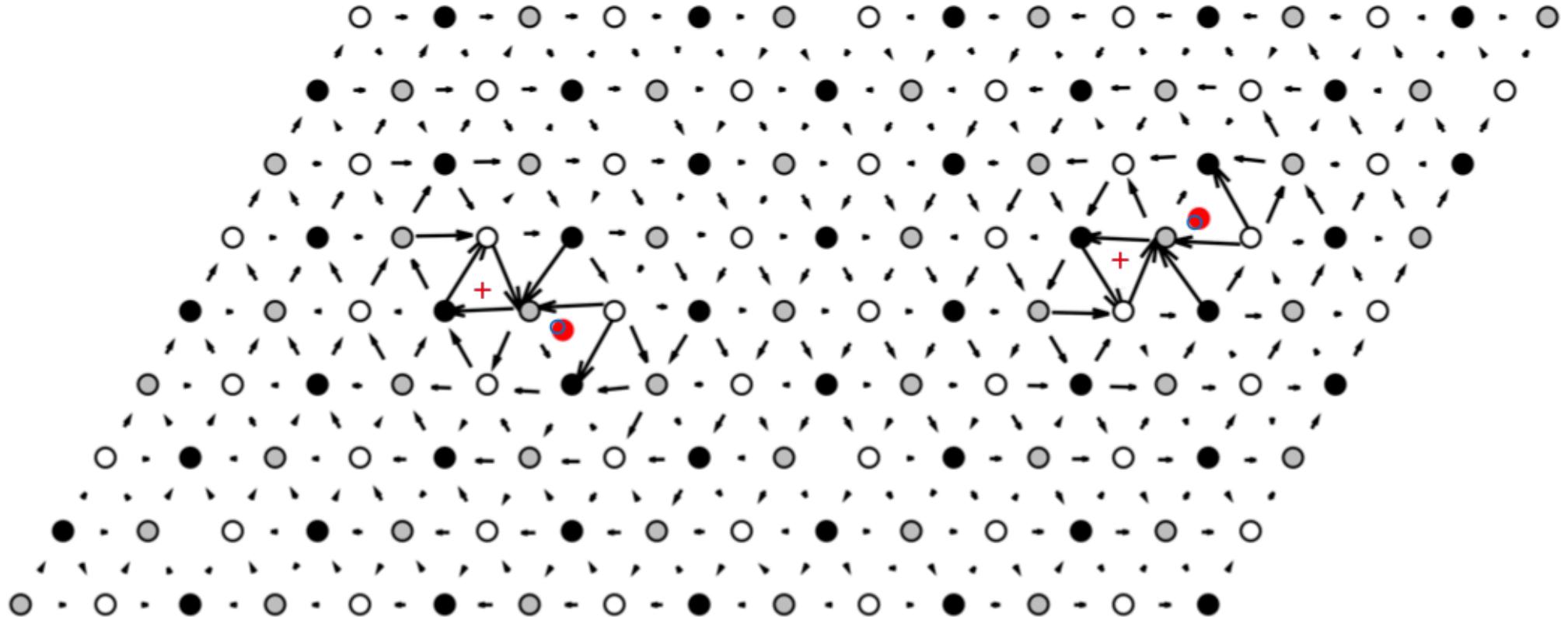
Initial  
Easy core dislocation  
O in position 1<sup>st</sup> – 4<sup>th</sup> and 6<sup>th</sup> NN

Final  
Hard core dislocation  
O in position 2<sup>nd</sup> NN

E = -1.83 eV

# Dislocation core-O interactions

Y. Zhao, L. Dezerald, J. Marian, Metals (2019)



Initial

Easy core dislocation  
O in position 5<sup>th</sup> NN

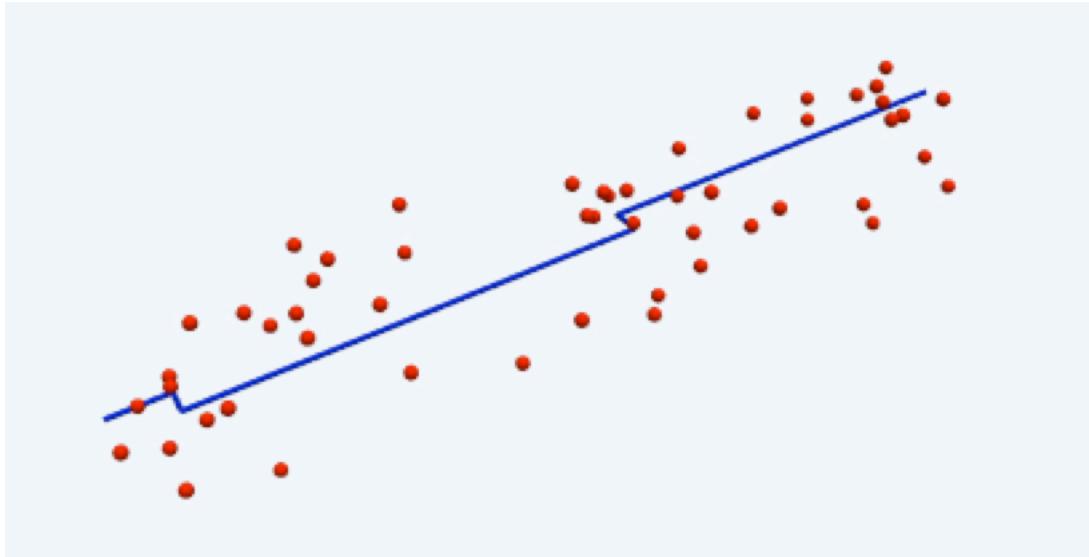
Final

Hard core dislocation  
O in position 5<sup>th</sup> NN

$E = -1.20 \text{ eV}$

# Upscaling with kMC

Preliminary results!

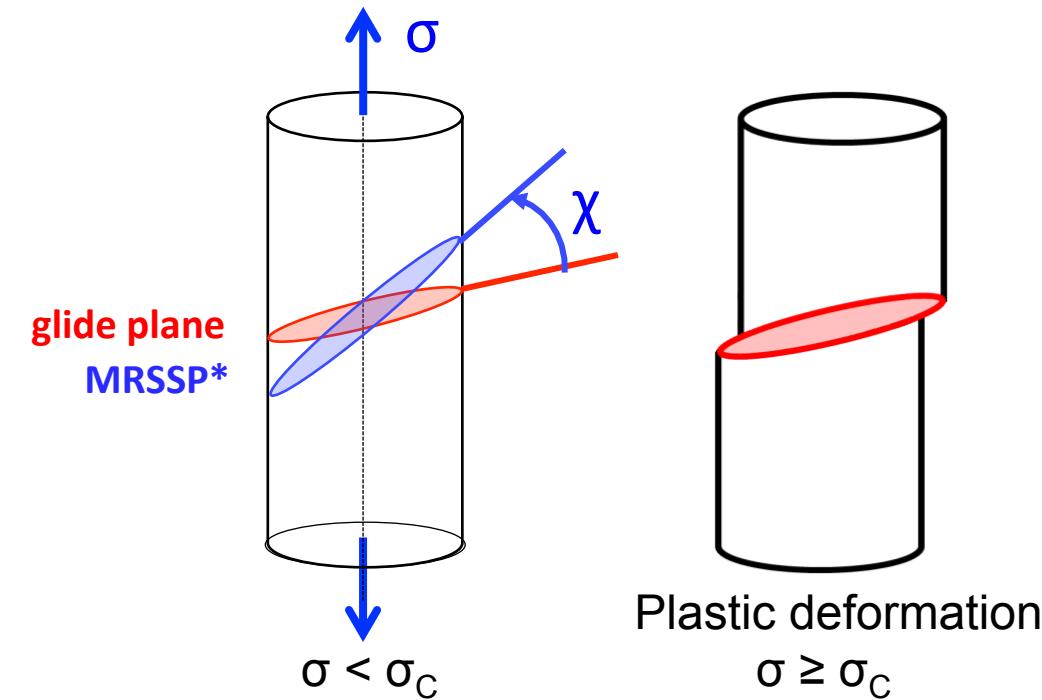


$\tau = 900 \text{ MPa}$   
 $T = 300 \text{ K}$

# Outline

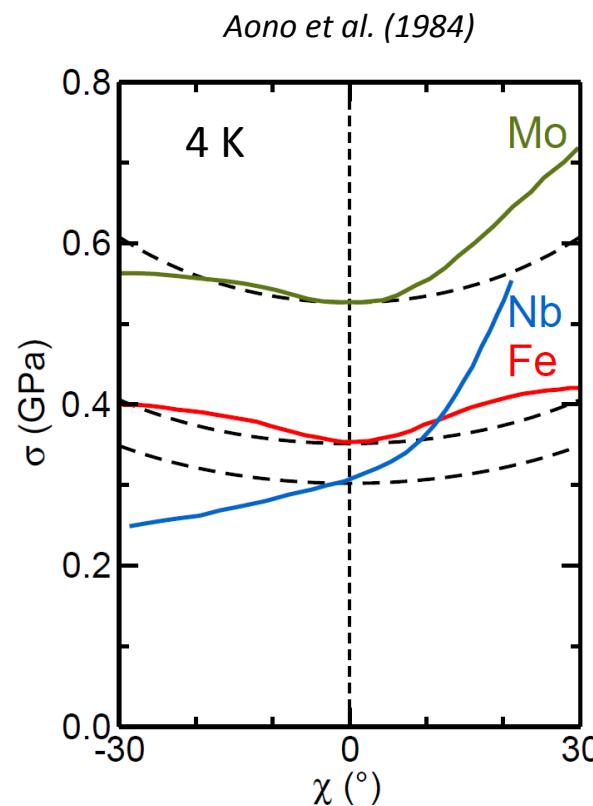
1. Dislocation-O coevolution in W
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*LabEx project for 2019-2020*

# Schmid law deviation in BCCs



**Schmid law:**  
Glide occurs in the glide plane when the resolved shear stress projected in the glide plane is superior to a constant value:

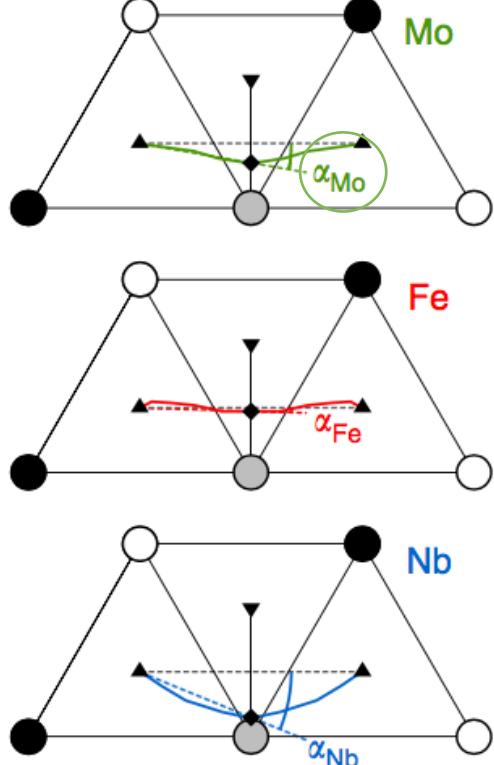
$$\sigma_c(\chi) = \frac{\sigma_c(0)}{\cos(\chi)}$$



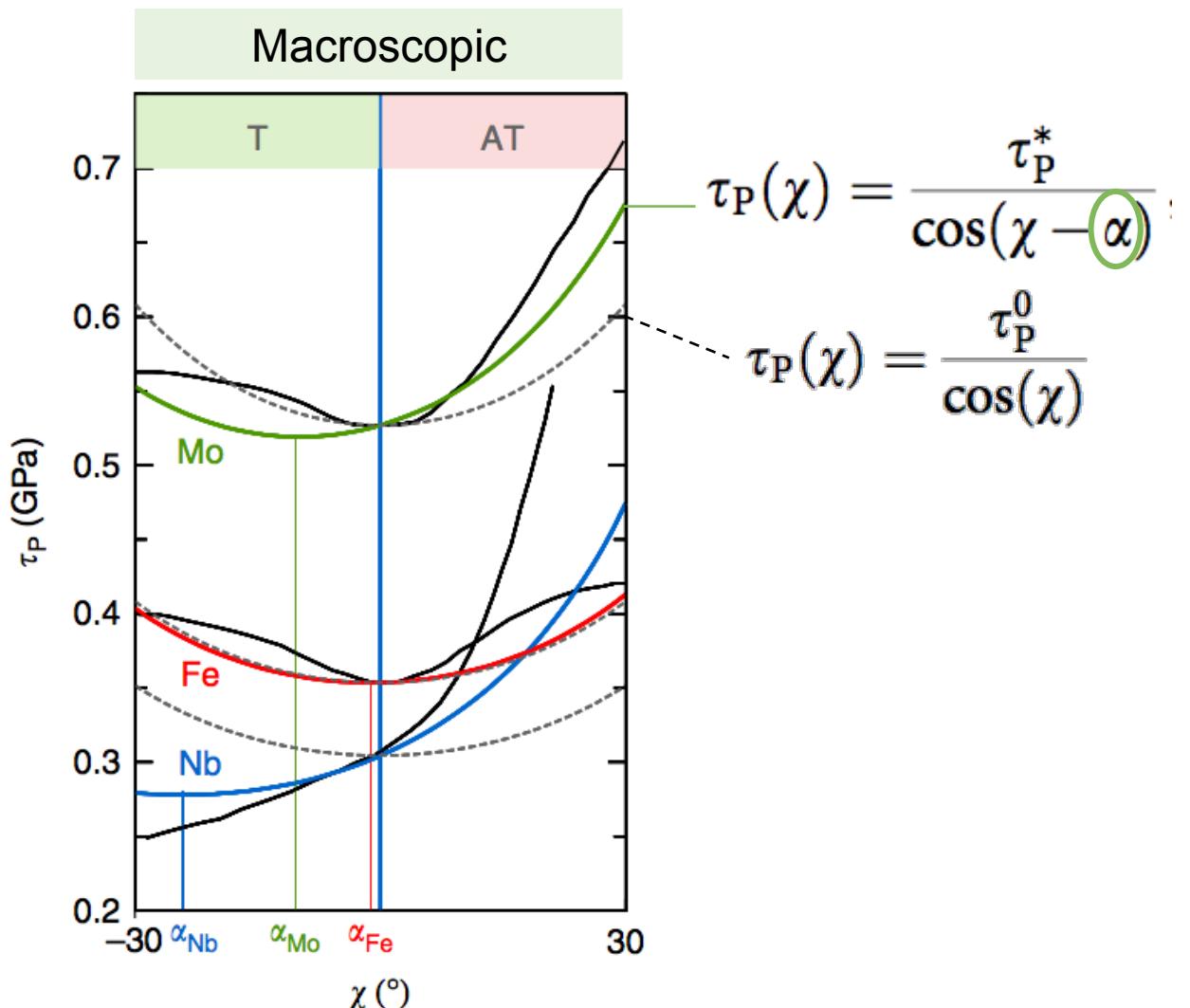
- Schmid law deviation
- metal-dependent

# Effect of shear stress

Atomic



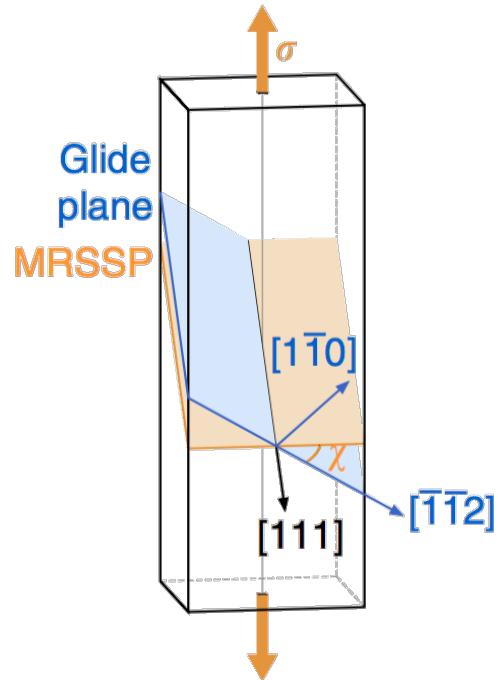
Macroscopic



Dezerald et al. Nat. Commun. (2016)

# Effect of non-glide stresses

Glide stress = shear stress (former DFT work)



In tensile tests, all components of stress tensor in dislocation frame are non-null

$$\Sigma(\tau, \chi) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \tau \\ 0 & \tau & 0 \end{pmatrix}$$

LabEx project: effect of other components on dislocation core? on Schmid law deviation?

Groger (Phil Mag 2014) : non glide stresses affect dislocation glide

$$\Sigma(\tau, \chi) = \begin{pmatrix} -\sigma & 0 & 0 \\ 0 & \sigma & \tau \\ 0 & \tau & 0 \end{pmatrix}$$

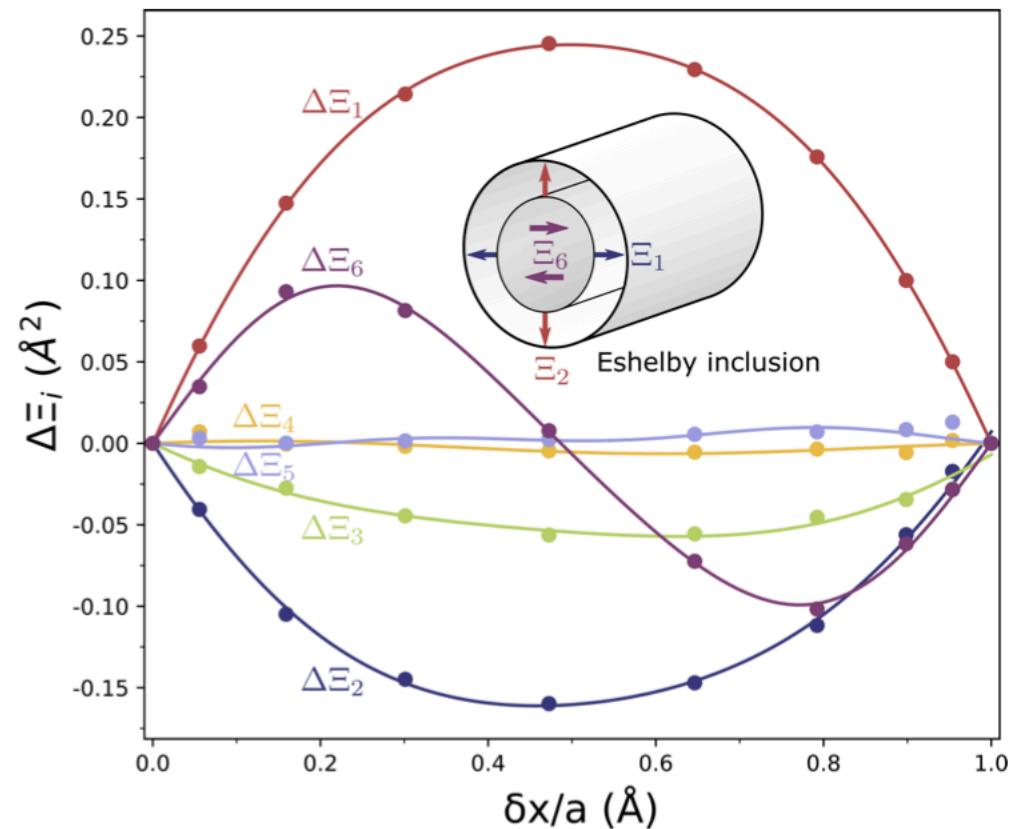
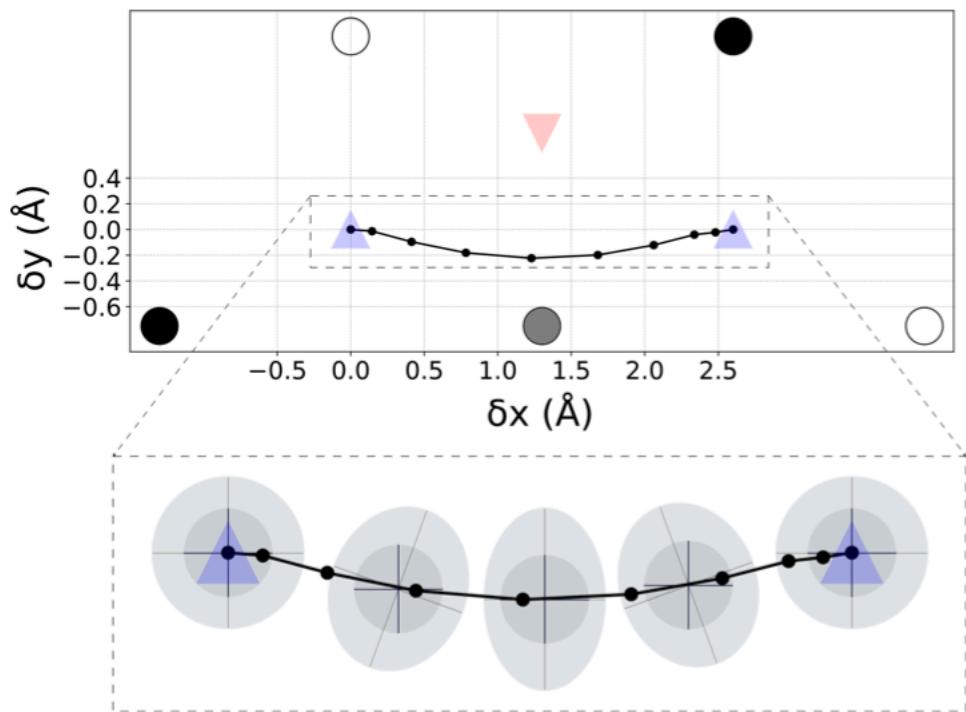
$$\tau_P(\chi, \sigma) = \frac{\tau_P^1 - \sigma(a_2 \sin(2\chi) + a_3 \cos(2\chi + \pi/6))}{\cos(\chi) + a_1 \cos(\chi + \pi/3)}$$

# Effect of non-glide stresses in W

$$\tau_P(\chi, \sigma) = \frac{\tau_P^1 - \sigma(a_2 \sin(2\chi) + a_3 \cos(2\chi + \pi/6))}{\cos(\chi) + a_1 \cos(\chi + \pi/3)}$$

effect of non-glide stresses  
eigenstrain

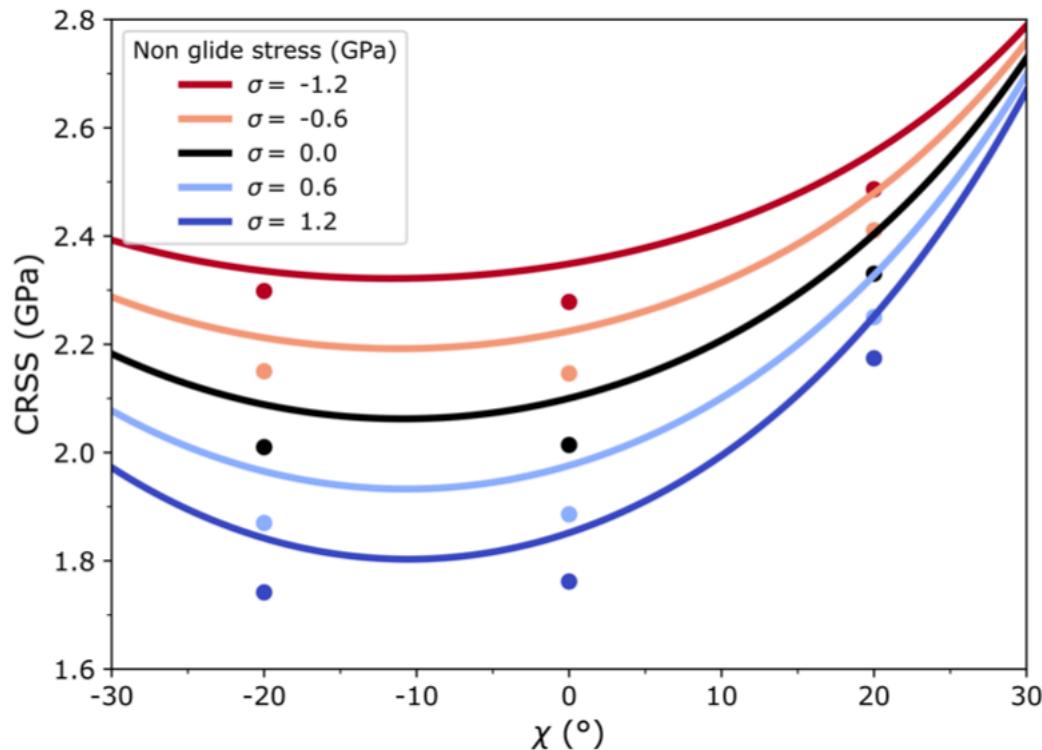
effect of shear stress  
trajectory



# Effect of non-glide stresses in W

$$\tau_P(\chi) = \frac{\tau_P^*}{\cos(\chi - \alpha)}$$

$$\tau_P(\chi, \sigma) = \frac{\tau_P^1 - \sigma(a_2 \sin(2\chi) + a_3 \cos(2\chi + \pi/6))}{\cos(\chi) + a_1 \cos(\chi + \pi/3)}$$

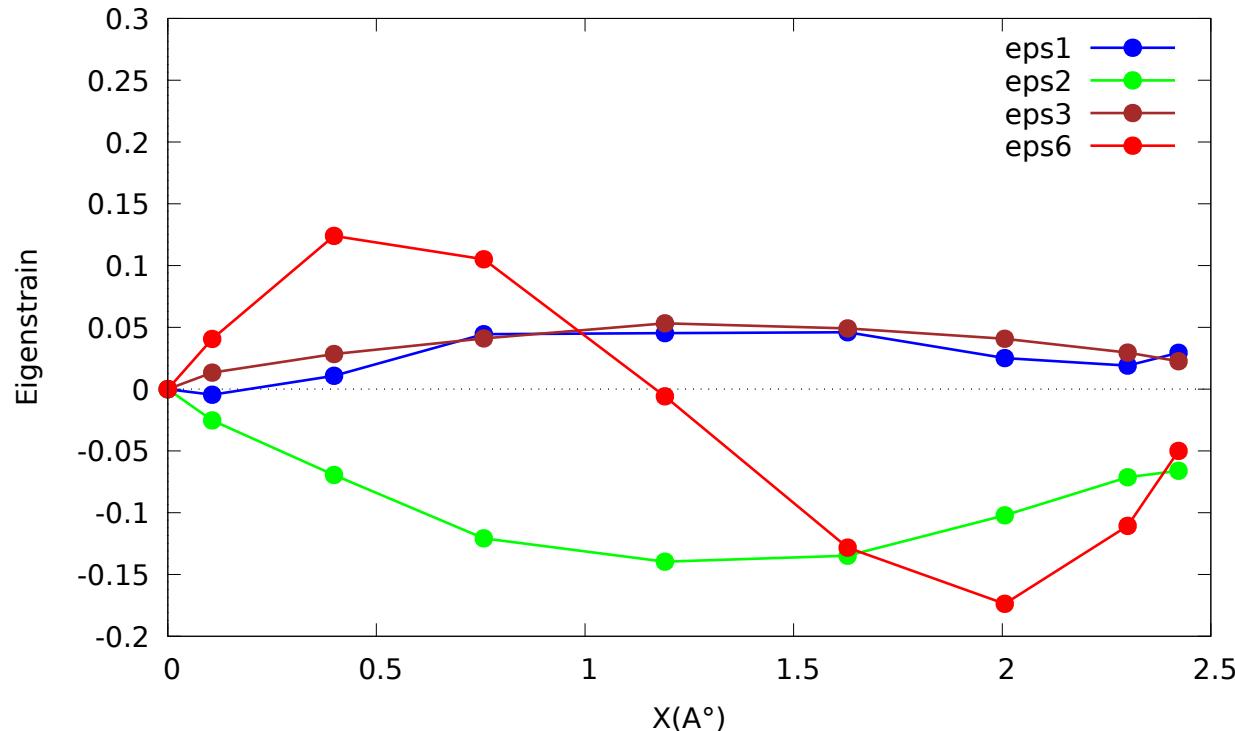


effect of non-glide stresses  
eigenstrain

effect of shear  
trajectory

Kraych et al. in preparation (2019)

# Effect of non-glide stresses in Mo



## Work in progress

- Finalize convergence parameters
- Link with Schmid law deviation
- Link with glide planes
- Comparison to experiments
- Extension to other BCC metals

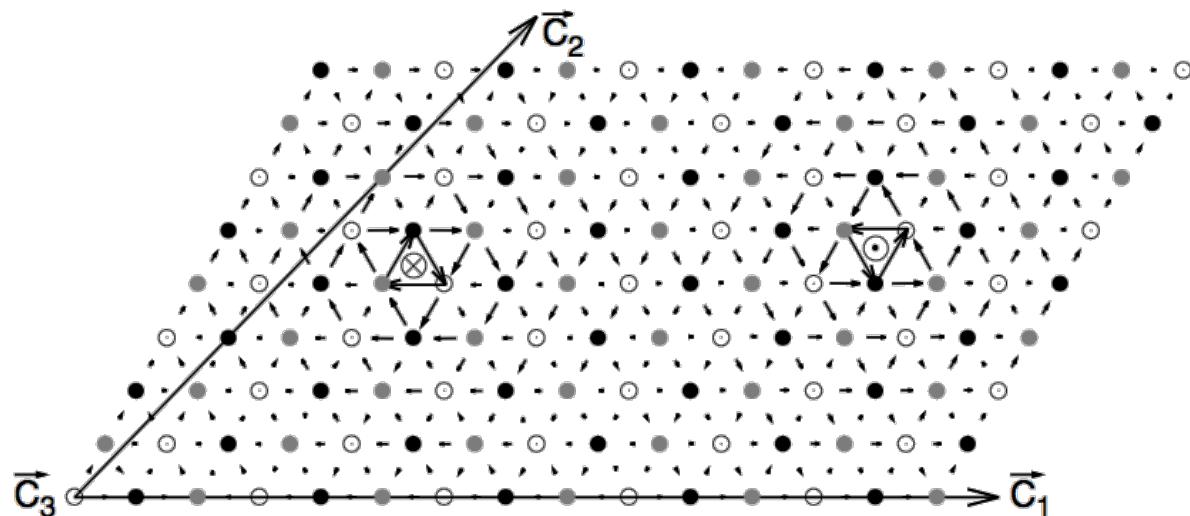
*Ph.D thesis of B. Ben Yahia*

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*LabEx project for 2019-2020*

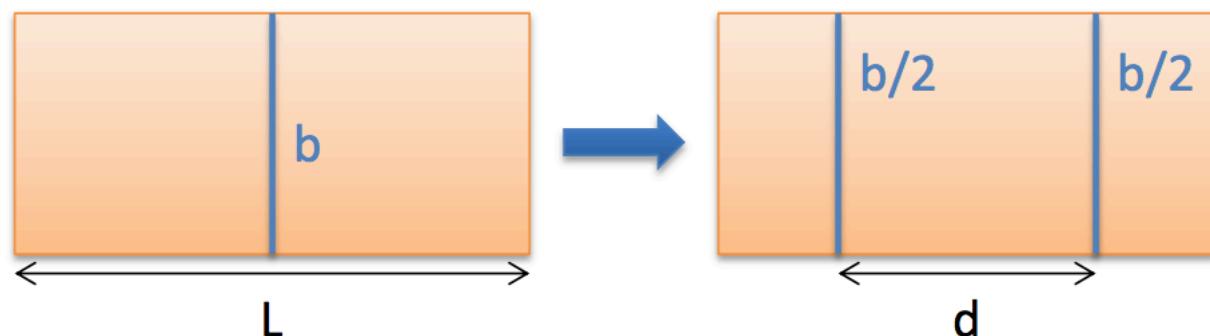
# Project for this year

## Ab initio modelling of dislocations in FCC metals



BCC metals

**Compact core**  
→ Dislocation dipole,  
135 atoms simulation cell

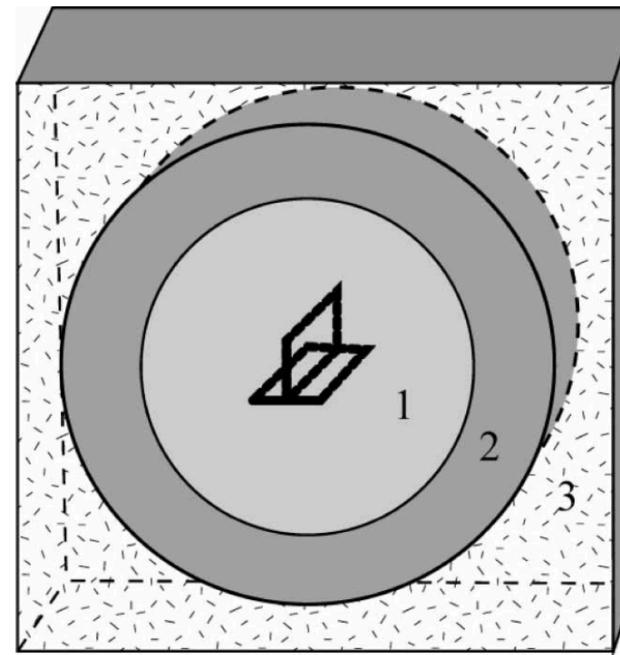
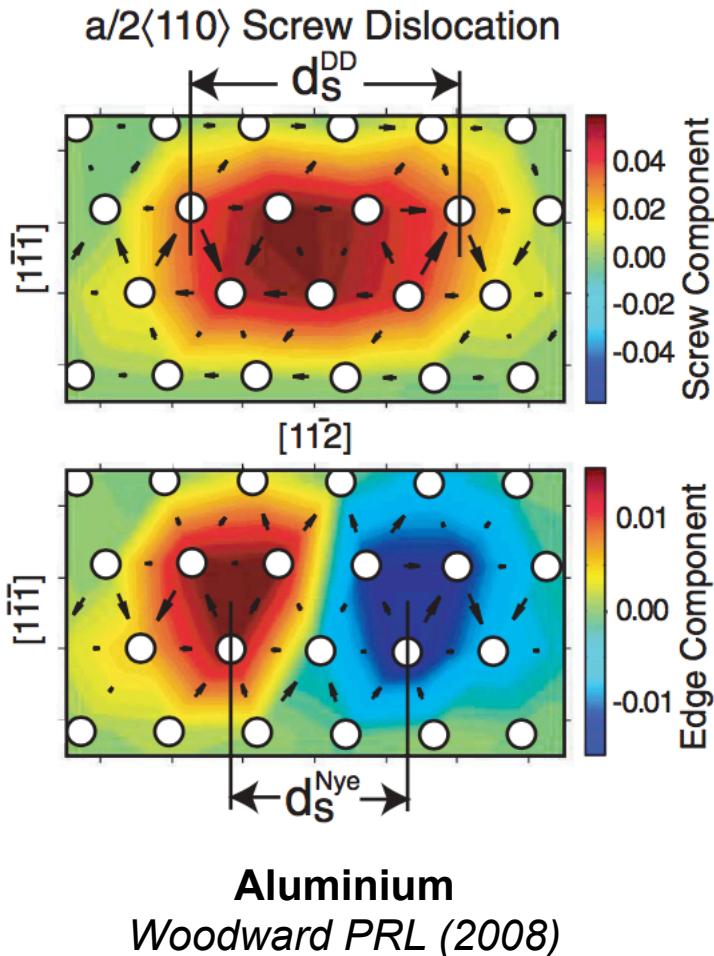


FCC metals

**Extended core**  
→ Other approach needed

# Project for this year

## Ab initio modelling of dislocations in FCC metals

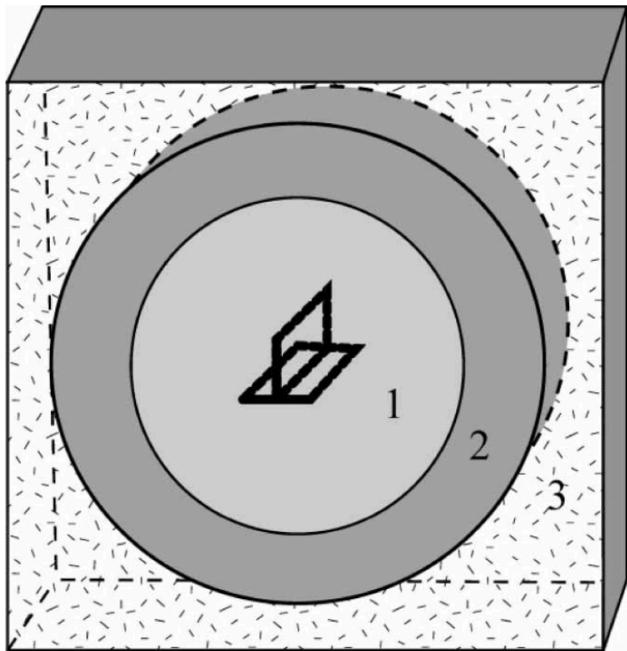


**Green functions boundary conditions**  
Still limited to small separation distances

**Project: adapt GFBC to partial dislocations**

# Project for this year

## Ab initio modelling of dislocations in FCC metals



- Adapt GFBC to partial dislocations
- Implement in VASP
- Applicable to any FCC metal
  - Austenitic Fe (TWIP)
  - $\gamma/\gamma'$
  - etc.
- Dislocation-solute interactions, input for larger scale models
- Collaboration: V. Taupin
- 2 year postdoc

# Conclusions

- Ab initio simulations of dislocations in BCC metals
  - Evidence trends/mechanisms at the atomic scale
  - Upscale with kMC or analytical models
- Collaborations with UCLA, CEA Saclay, ILM Lyon
- Conferences:  
  MMM (Osaka, J. Marian), Hermes Workshop (London, B. Ben Yahia)
- Future conferences:  
  RNM (Nancy, BBY), Euromat (Stockholm, BBY), Dislocations (Haifa, LD)
- Papers: W-O : Metals (2019) + 1 in preparation (kMC)
- Project: Develop method to investigate dislocations in FCC metals with DFT
  - Collaboration with V. Taupin
  - 1 postdoc