# The Stress Dependence of Cross-slip in FCC Nickel

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Tuesday October 7th, 2014

7th International Conference on Multiscale Materials Modeling

Berkeley, CA

# Contents


Introduction to cross-slip

- Screw dislocations and partials
- Cross-slip mechanisms
- Stress components

Molecular statics

- String method
- Reparametrization with trimming

Results

- Energy barriers
- Which mechanism dominates?
- Activation volumes

Looking forward

- Incorporation into dislocation dynamics

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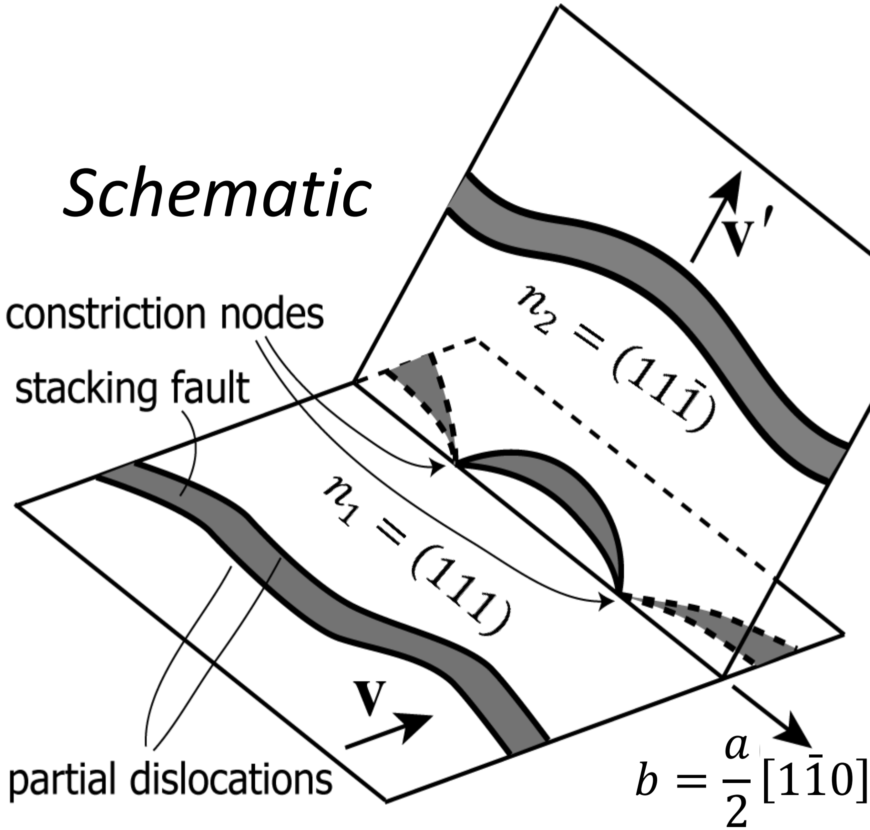
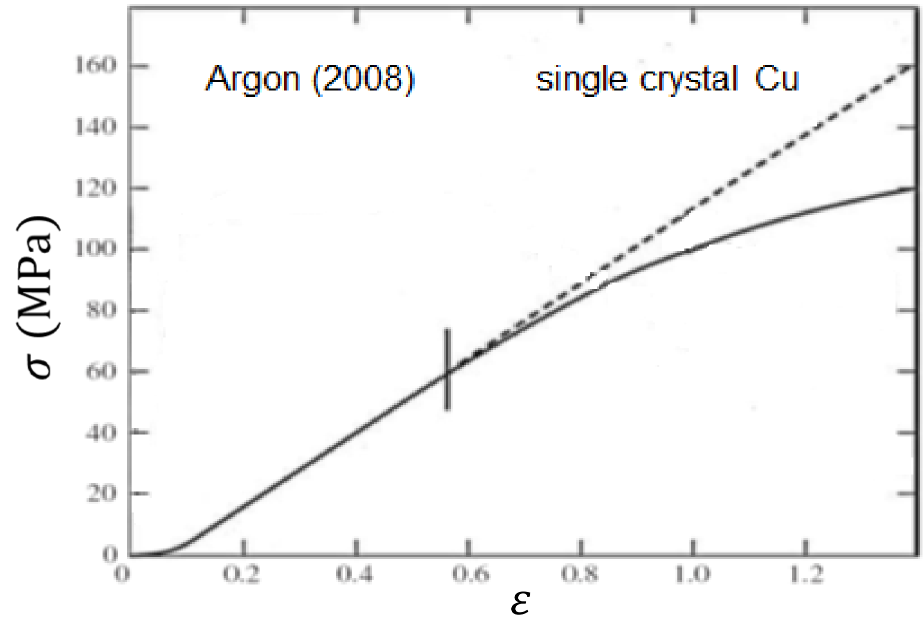
# Partial Dislocations and Cross-slip in FCC Metals



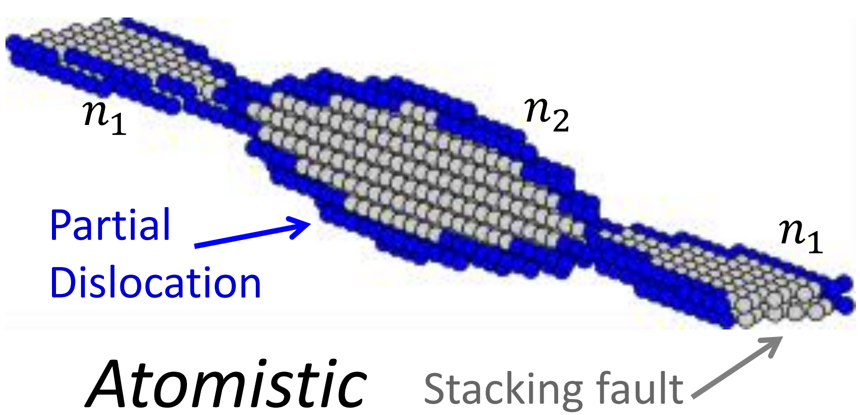




Cross-slip is believed to be important for:

- Dislocation multiplication
- Strain hardening
- Dynamic recovery (onset of stage III)
- Pattern formation

Goal: input for DD simulations

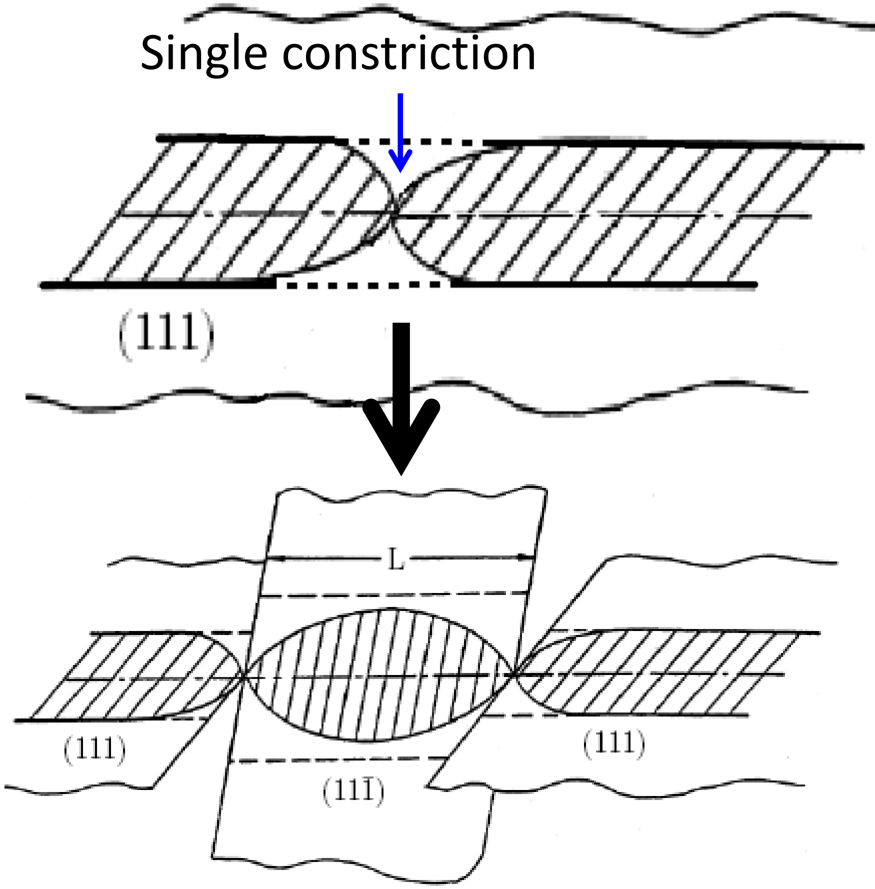
$$j = \nu \frac{l}{l_0} exp\left(\frac{-E(\sigma_{ij})}{k_B T}\right)$$





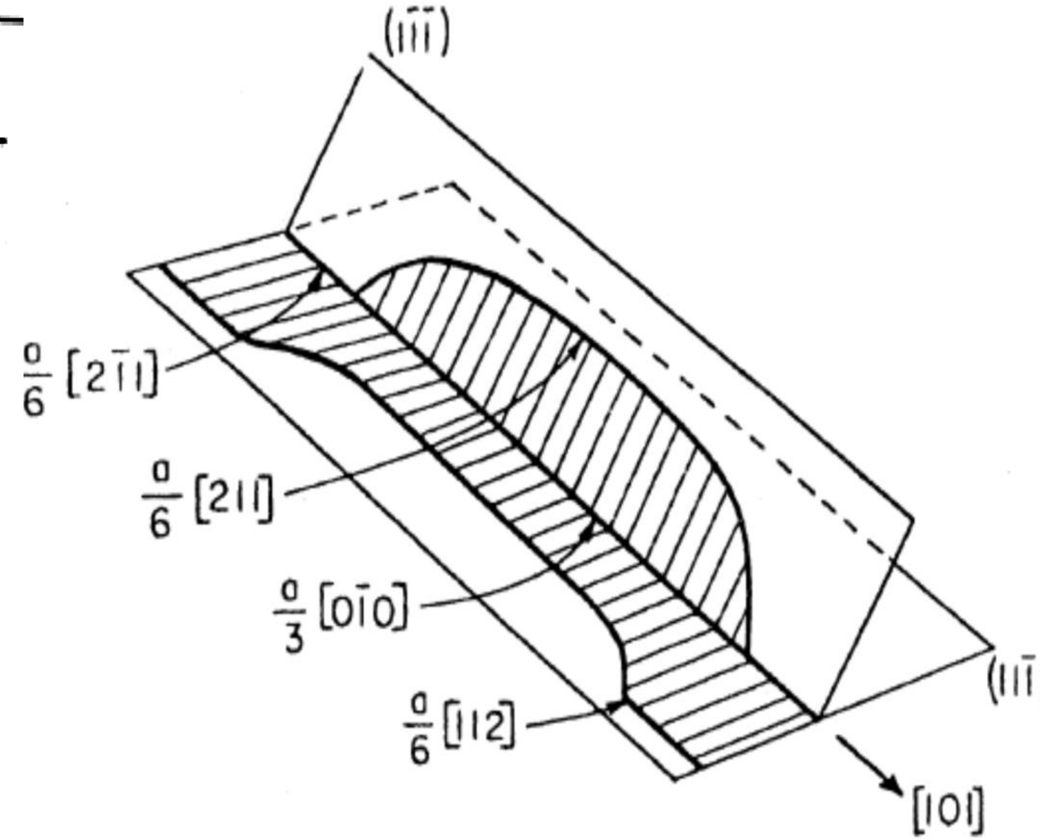

Kubin et al., Solid State Phenomena, **23-24**, 455 (1992).

# Cross-slip Mechanisms




**Friedel-Escaig** (FE)

Forms a single constriction to initiate cross-slip

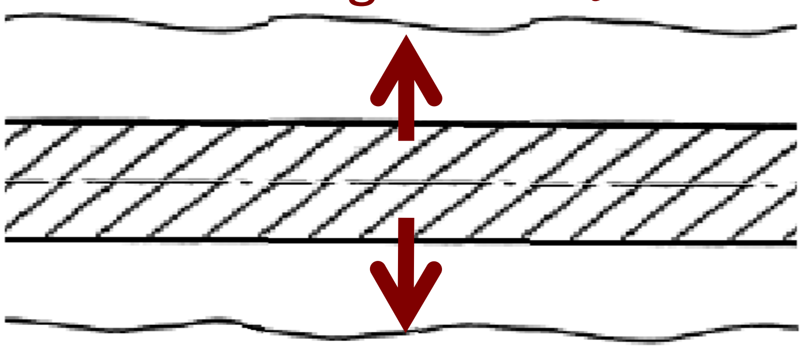



**Fleischer** (F)

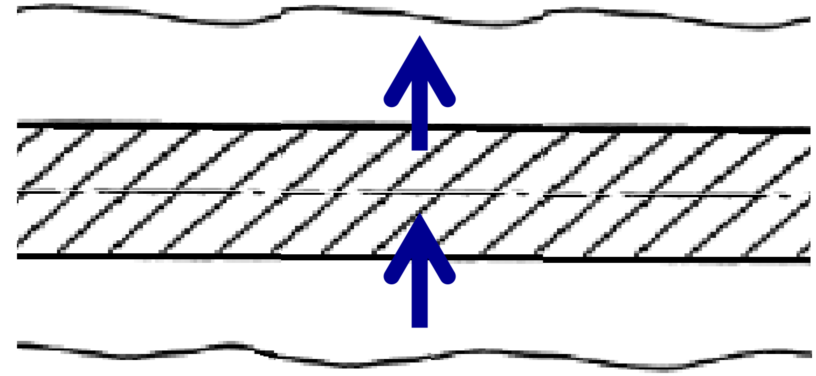
No constriction formed leading to 3D structure

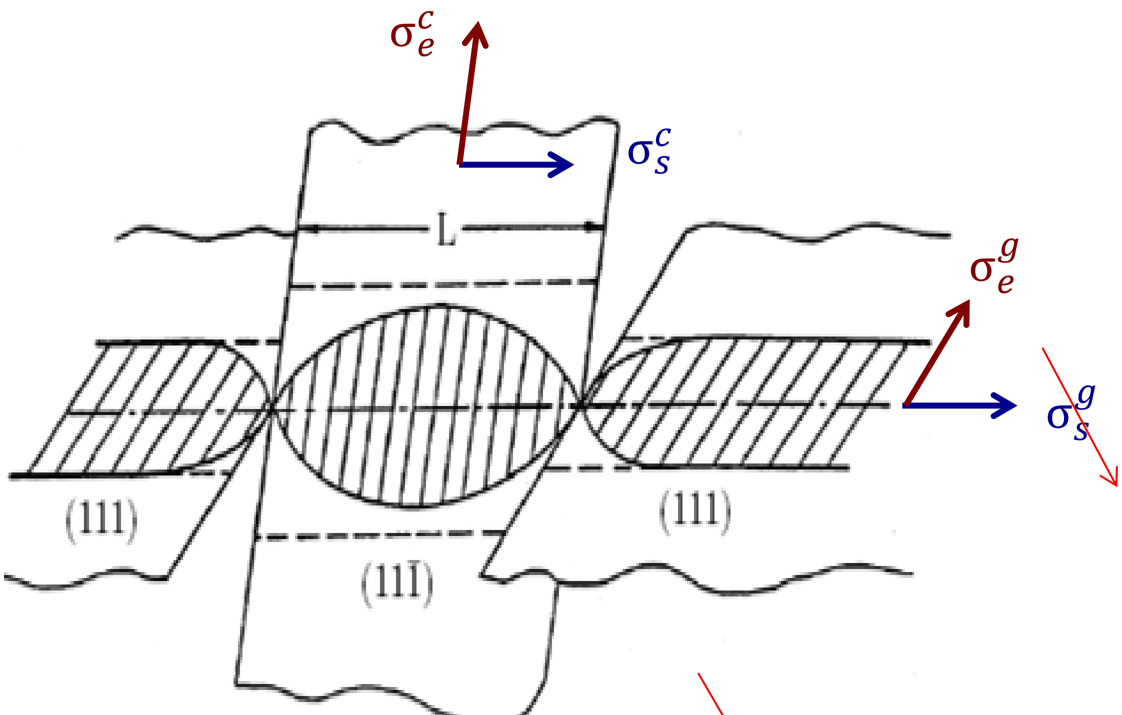
# Stress Components

Escaig stress $\sigma_e$



Schmid stress $\sigma_s$






$E_b(\sigma_s^g, \sigma_e^g, \sigma_s^c, \sigma_e^c)$

- Assume Schmid stress on glide plane is zero (i.e. dislocation is not moving)
- Stress in 200 Mpa increments from 0 to 1000 MPa
- 6x6x6 = 216 stress configurations with multiple stresses

Review by Puschl, Prog. Mater. Sci. **47**, 415 (2002)

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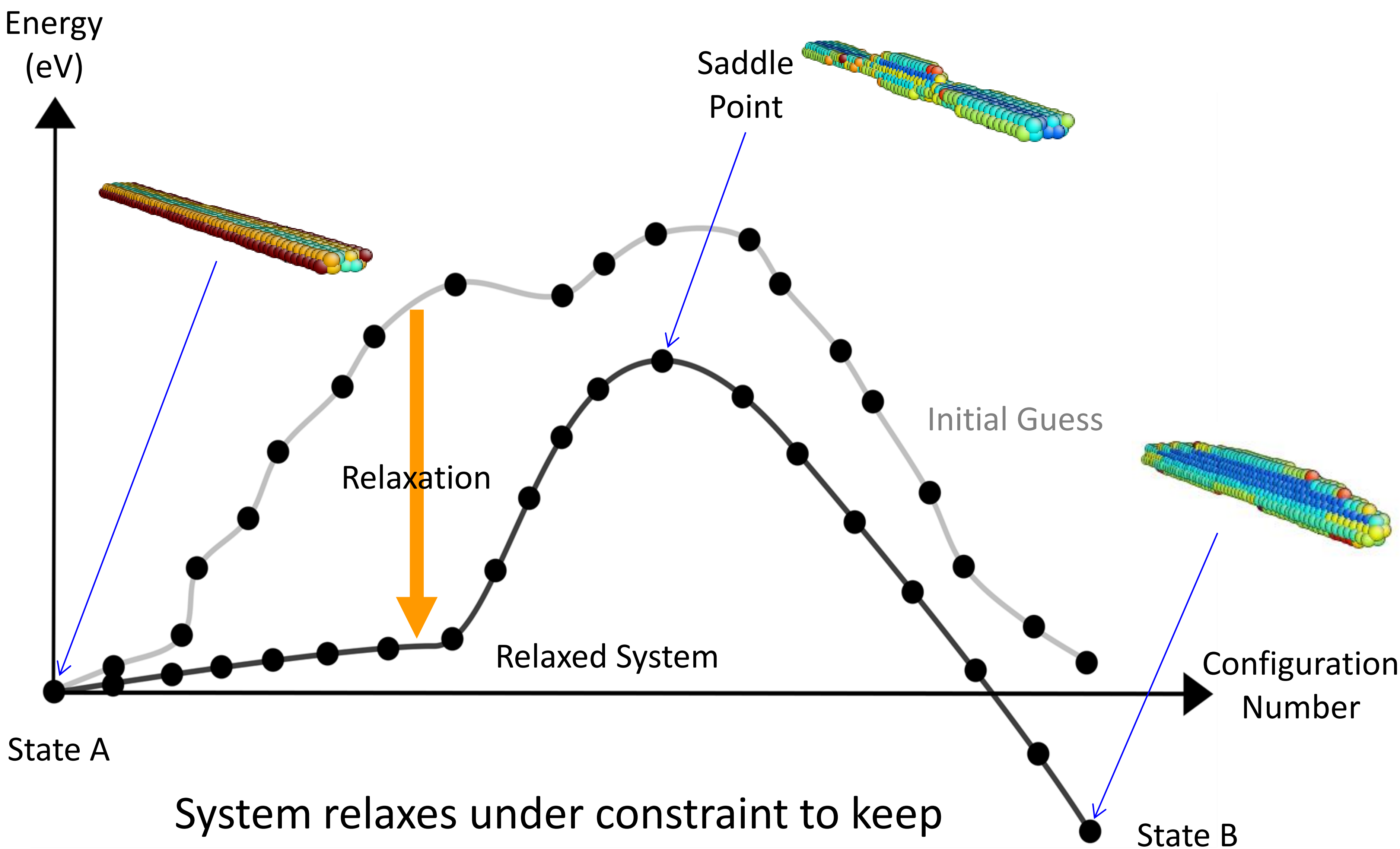
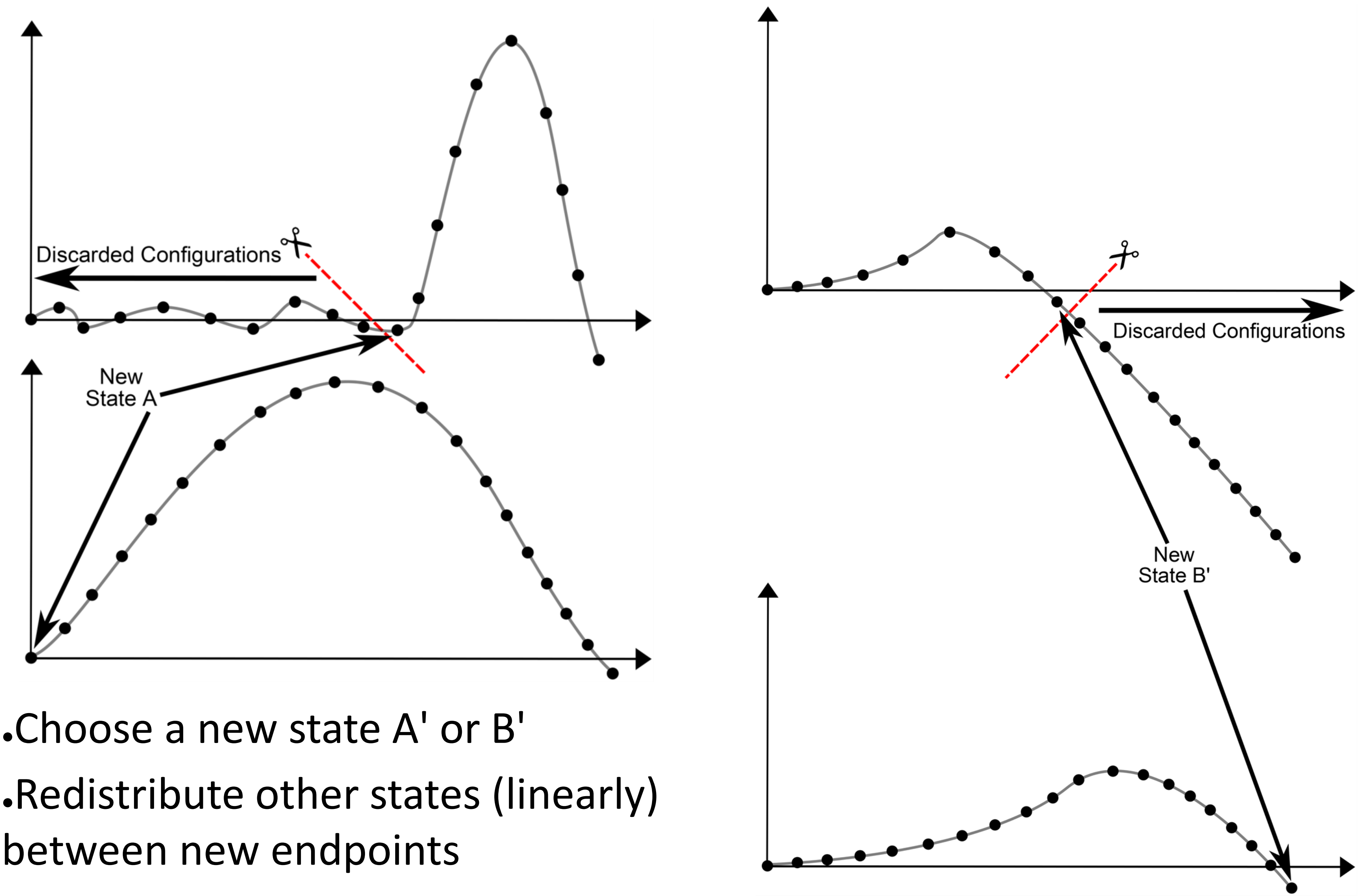
# Molecular Statics and the String Method




System relaxes under constraint to keep configurations equally separated

# Reparametrization with Trimming Algorithm




- Choose a new state A' or B'
- Redistribute other states (linearly) between new endpoints
- Relax using conjugate gradient technique

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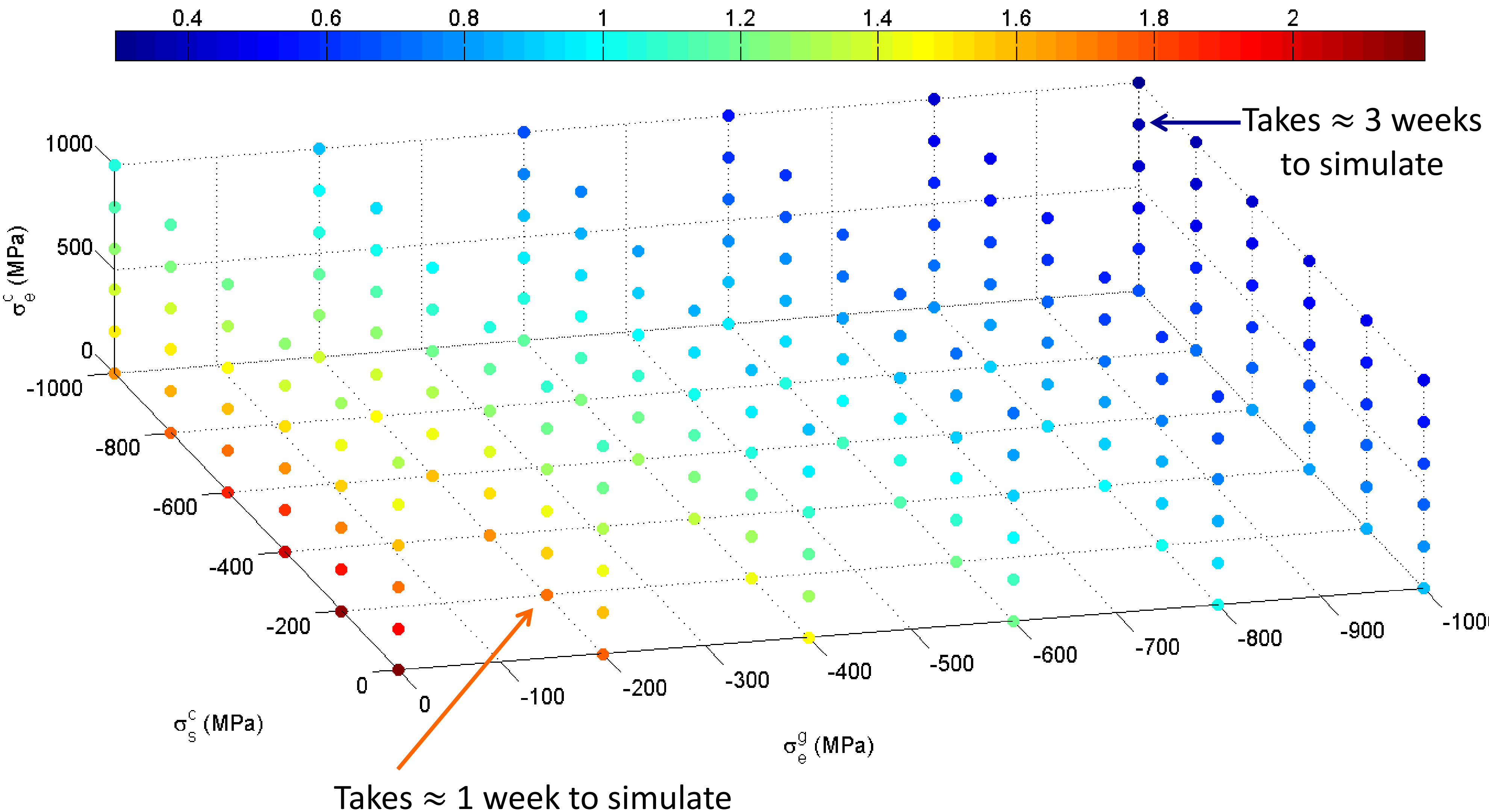
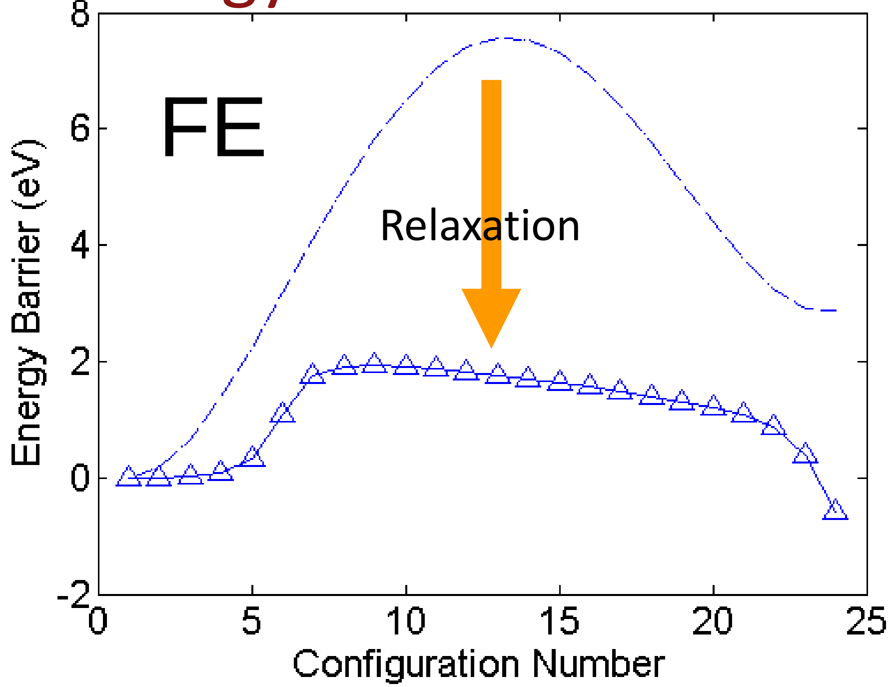
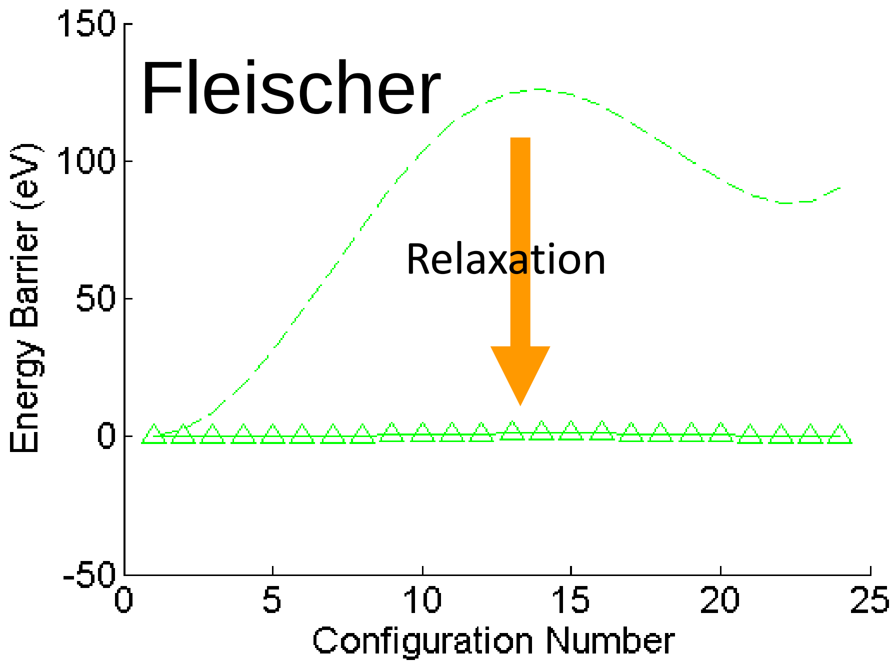
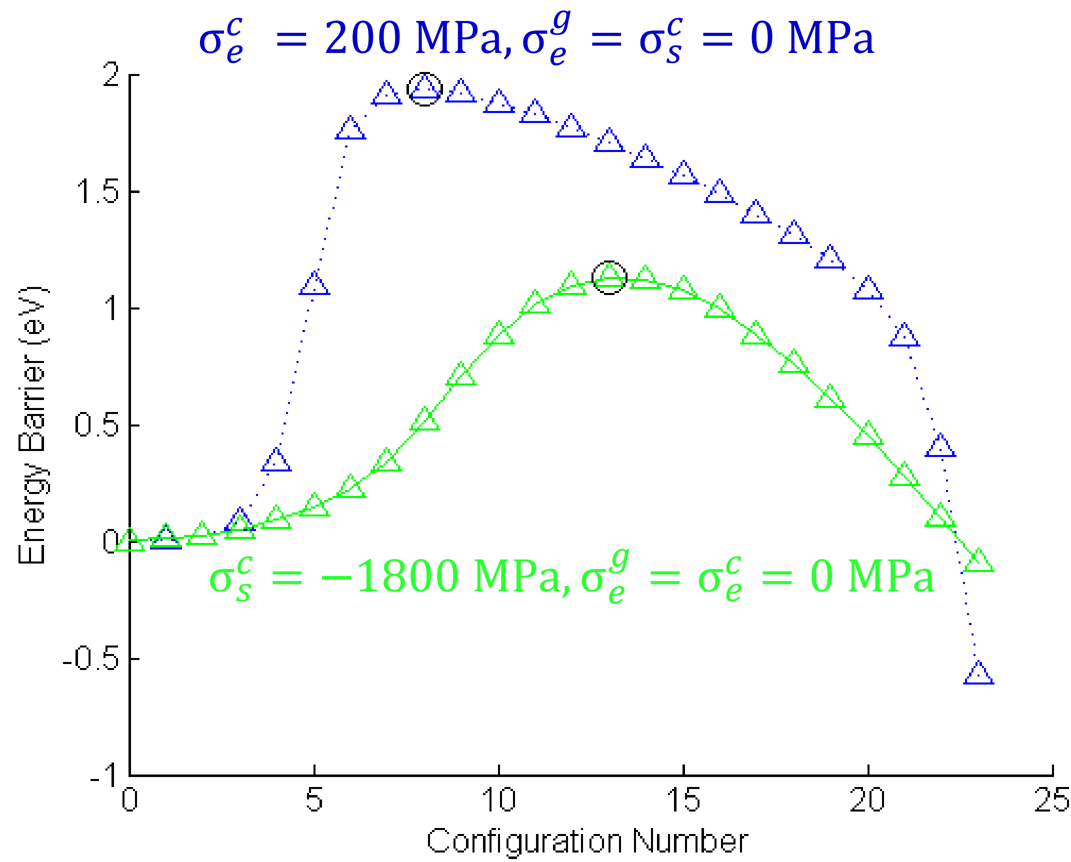
# Raw Data Points for FE Mechanism



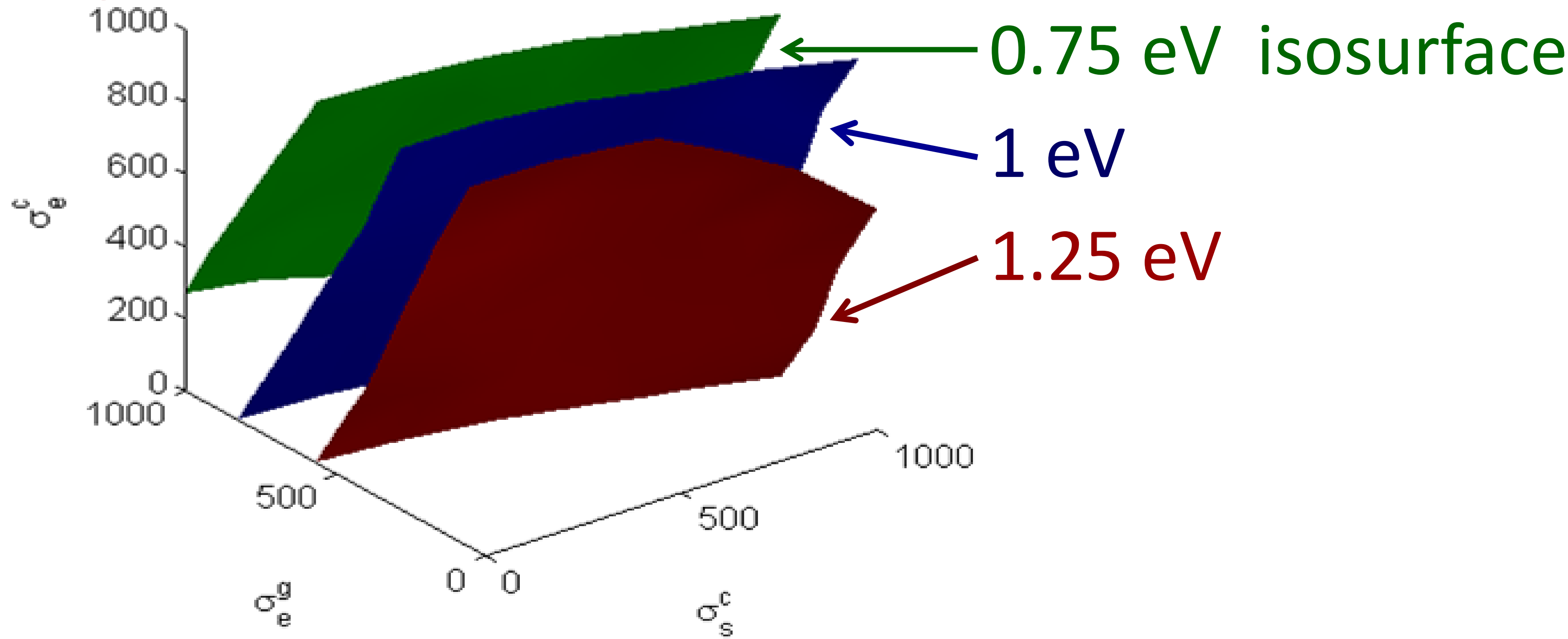
# Energy Barriers for Both Mechanisms

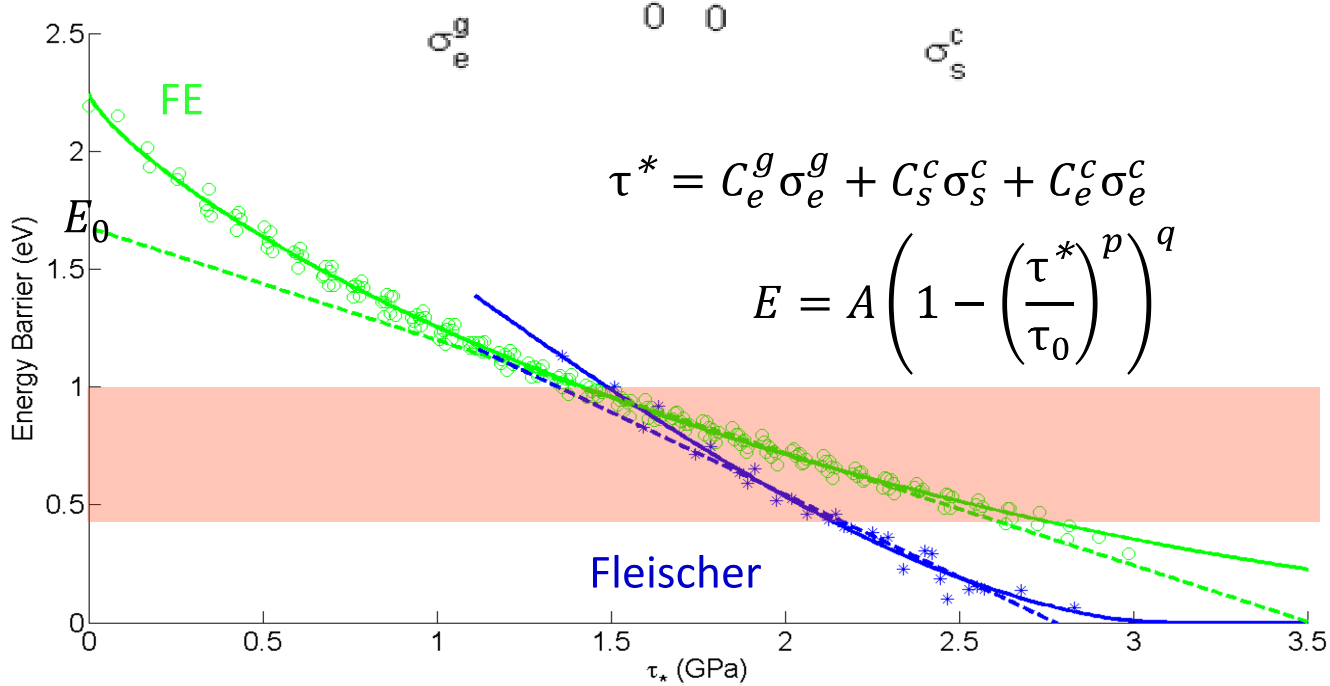


# Fitting Functions



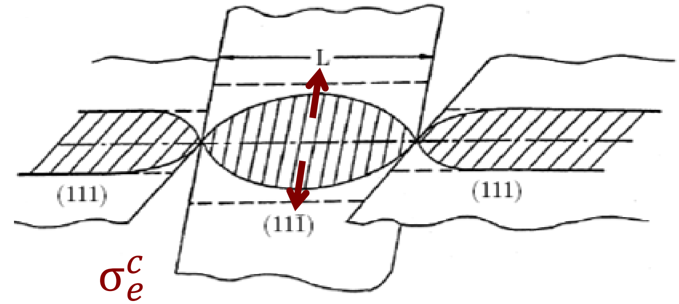




$$\tau^* = C_e^g \sigma_e^g + C_s^c \sigma_s^c + C_e^c \sigma_e^c$$

$$E = A\left(1 - \left(\frac{\tau^*}{\tau_0}\right)^p\right)^q$$

| | FE | Fleischer |
|---|---|---|
| $C_e^g$ | -1.68 | -0.96 |
| $C_s^c$ | -0.42 | -0.76 |
| $C_e^c$ | 0.88 | 0.69 |

Energy barrier region of interest




# Which Mechanism Dominates?

Using Linear Fits

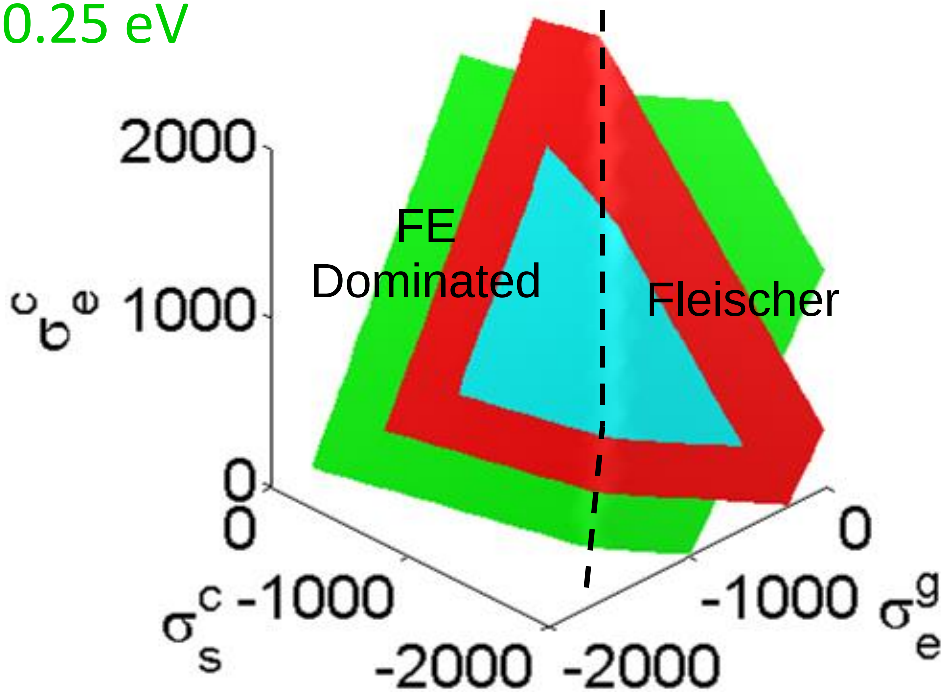
Boundary Between Two Mechanisms

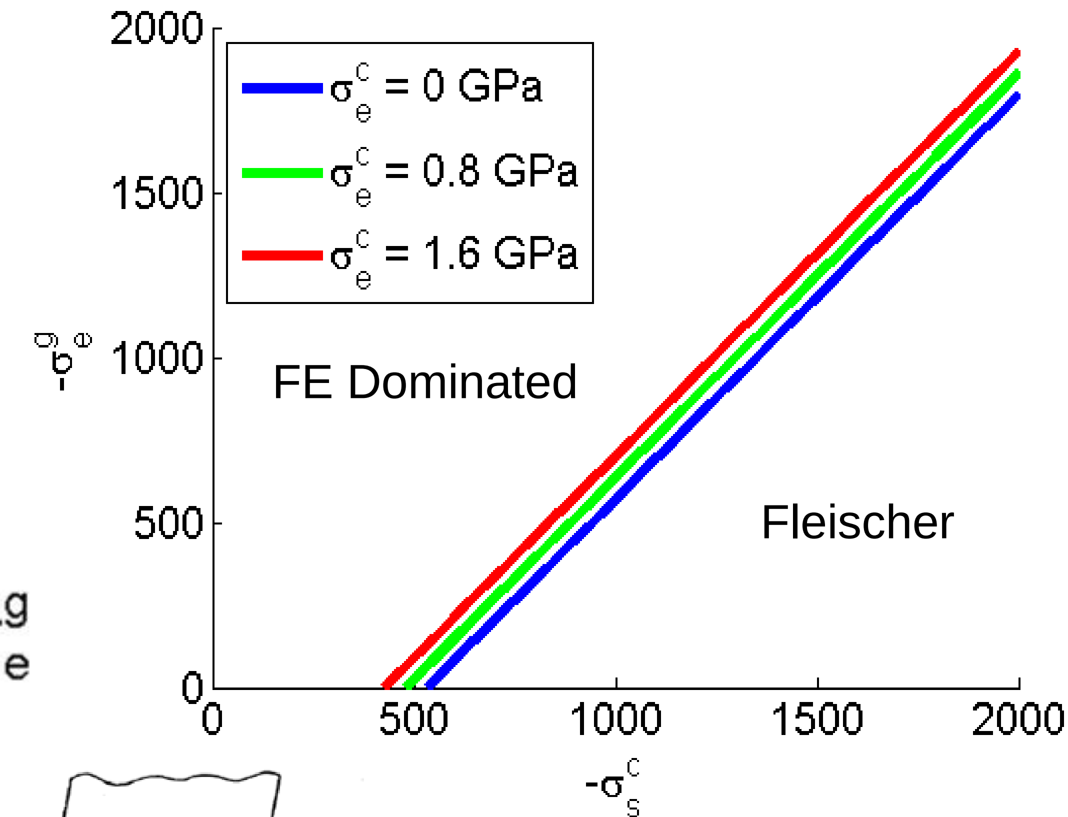
1.25 eV isosurface

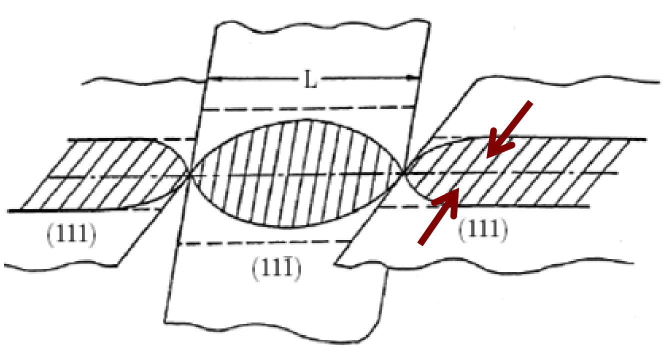
0.75 eV

0.25 eV

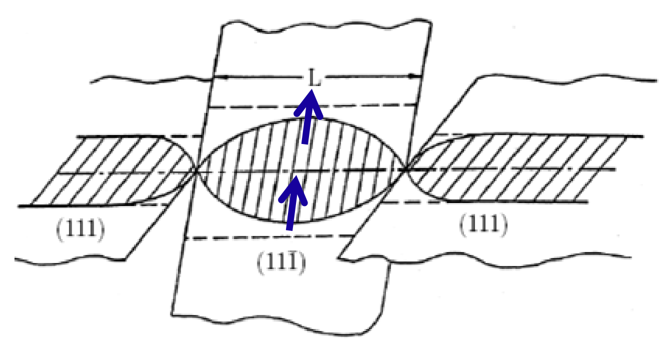
Minimum Energy Barrier




Larger $\sigma_e^g$ → FE Dominates




Larger $\sigma_s^c$ → Fleischer Dominates

# Activation Volume

$$\Omega = -\left(\frac{dE}{d\tau}\right) \longrightarrow \Omega_{ij} = -\left(\frac{dE}{d\sigma_{ij}}\right)$$

Activation volume is a tensor

$$\boldsymbol{\Omega} = \begin{bmatrix} 1.77 & 1.06 & -2.49 \\ 1.06 & 0.35 & -1.07 \\ -2.49 & -1.07 & -2.12 \end{bmatrix} b^3$$

One activation volume tensor for $b = \frac{a}{2}[1\bar{1}0]$ and $n = (111)$

↓

Cross-slip rate can be approximated with Arrhenius relation

$$\tau^* = C_e^g \sigma_e^g + C_s^c \sigma_s^c + C_e^c \sigma_e^c$$

↓

$$E = E_0(1 - \tau^*)$$

↓

$$E = E_0 - E_0 \tau^*$$

↓

$$E = E_0 - \Omega_{ij}\sigma_{ij}$$

$$j = \nu \frac{l}{l_0} exp\left(\frac{-\left(E_0 - \sigma_{ij}\Omega_{ij}\right)}{k_B T}\right)$$

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# Looking Forward to Dislocation Dynamics

- Goal is to incorporate cross-slip in dislocation dynamics (DD) simulations
- Can choose linear equation fit ⟶ $j = \nu \frac{l}{l_0} exp\left(\frac{-(E_0 - \sigma_{ij}\Omega_{ij})}{k_B T}\right)$
- Can choose exponential equation fit ($p \neq 1, q \neq 1$)

↓

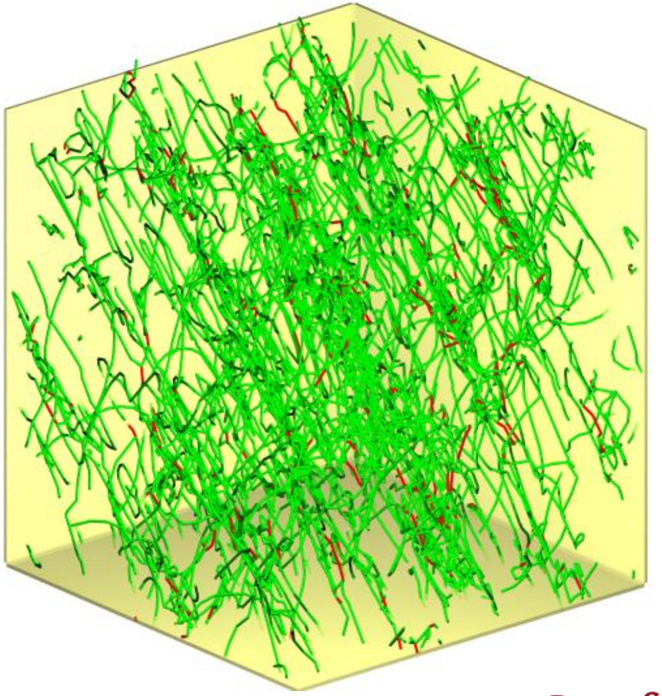
$$\tau^* = C_e^g \sigma_e^g + C_s^c \sigma_s^c + C_e^c \sigma_e^c$$

↓

$$E = A\left(1 - \left(\frac{\tau^*}{\tau_0}\right)^p\right)^q$$

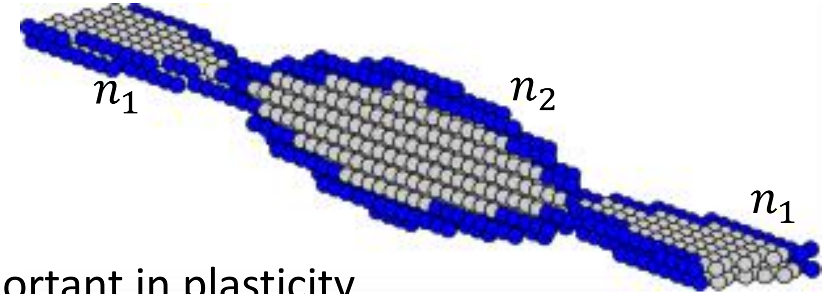
↓

$$j = \nu \frac{l}{l_0} exp\left(\frac{-E(\tau^*)}{k_B T}\right)$$



Taken from llnl.gov

2 cross-slip mechanisms means 2 fits!




# Summary

Cross-slip is important in plasticity

- Need a model for DD simulations

Simulated many stress configurations to find energy barriers

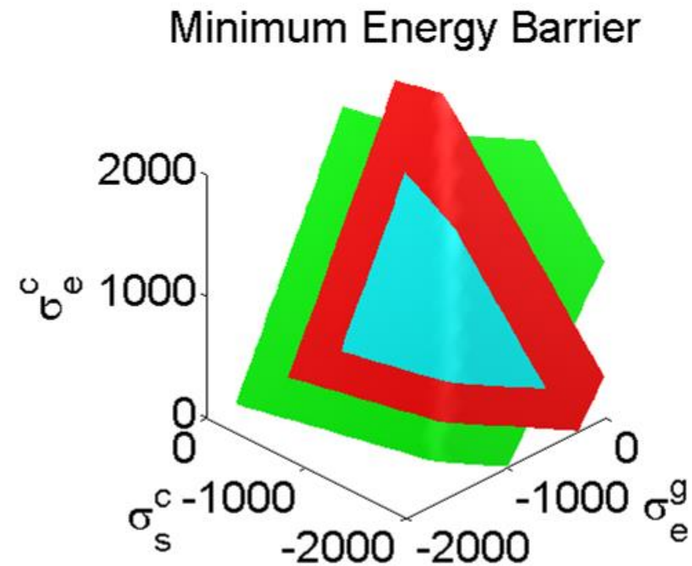
- Explored FE and Fleischer mechanisms

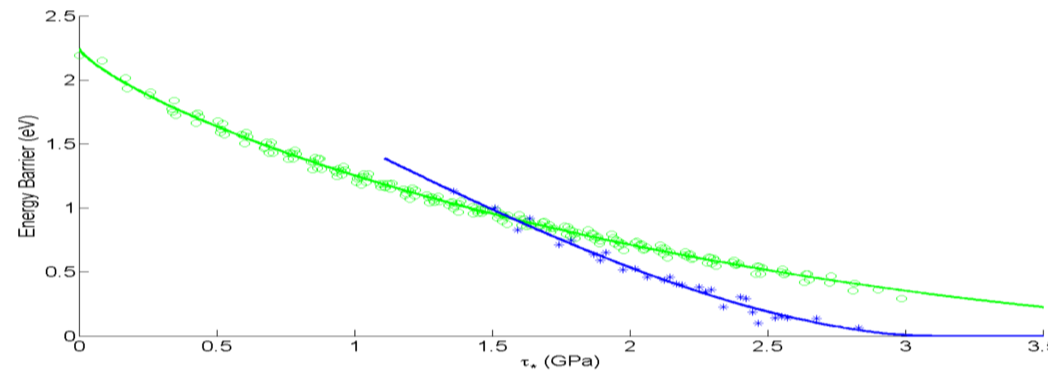
Fit data to an “effective stress”

- Even simple fits captured trends

Found the activation volume tensors for FE and Fleischer

- Can be incorporated into DD simulations




**Further reading:**


Keonwook Kang, Jie Yin and Wei Cai. *Journal of the Mechanics and Physics of Solids.* **62**, 181 (2014).

William Kuykendall and Wei Cai. “The Stress Dependence of Cross-slip in Nickel.” *In preparation*.



**Funding Acknowledgment**

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under award No. DE-SC0010412.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