MCP@60

Pembroke College Cambridge
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SLIP SLIDING AWAY

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TCM, Cavendish Laboratory 1994

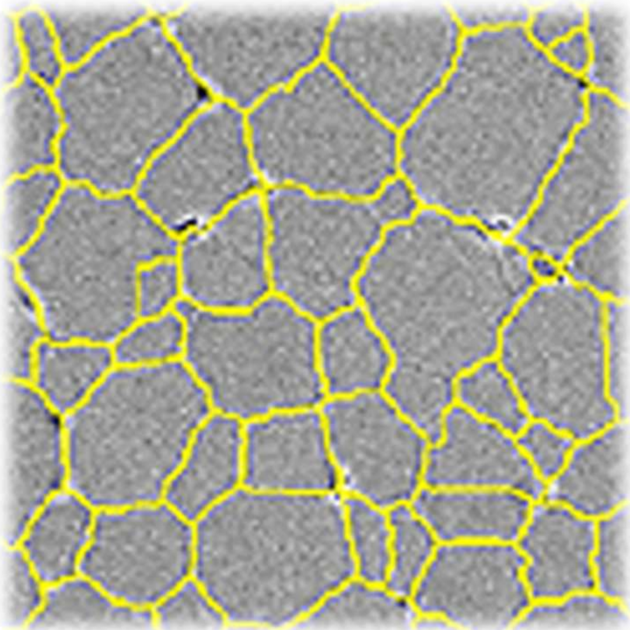
"Do whatever you want, provide you do some GOOD SCIENCE"

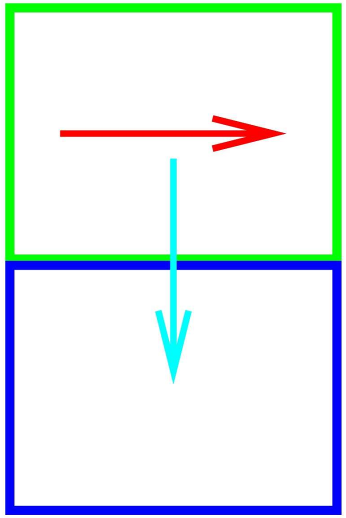
M.C. Payne, Tuesday 3 May 1994

"There is a directory with some data on grain boundaries…"

GRAIN BOUNDARY SLIDING

Any plastic shear displacement **parallel** to the boundary interface that occurs in response to external forces





MIGRATION

Motion of the interface between the two grains in the direction of the interface **normal**

GRAIN BOUNDARY SLIDING plays an important role in the **deformation** and **fracture** of **polycrystals** and affects their **strength** and **reliability**, especially at **high temperature**

- ***How quickly does a given material distort under stress? How is this rate affected by temperature?***

- ***What processes occur as the material ages under repeated distortions that eventually lead to its fracture and failure?***

GRAIN BOUNDARY SLIDING plays an important role in the **deformation** and **fracture** of **polycrystals** and affects their **strength** and **reliability**, especially at **high temperature**

- **to predict and prevent damage**
- **to design materials that resist mechanical aging**

GOAL

To get a detailed picture at the microscopic level of the processes that occur during the sliding, as a function of material, boundary geometry, local order and presence of defects, and to evaluate the effects of temperature and strain rate

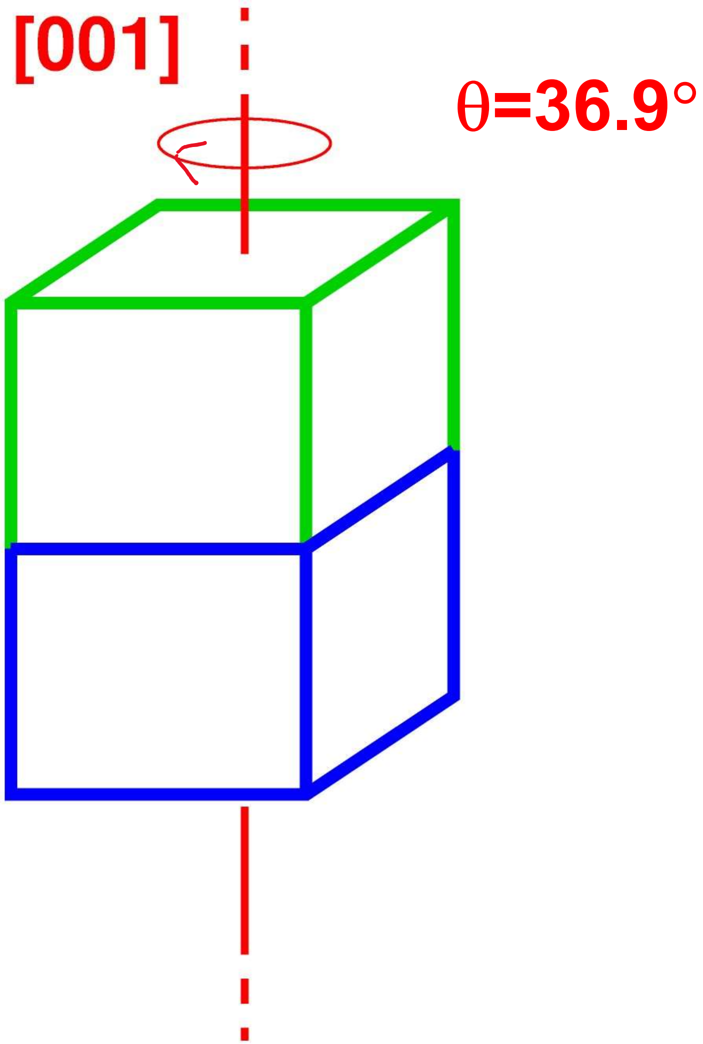
TOOL

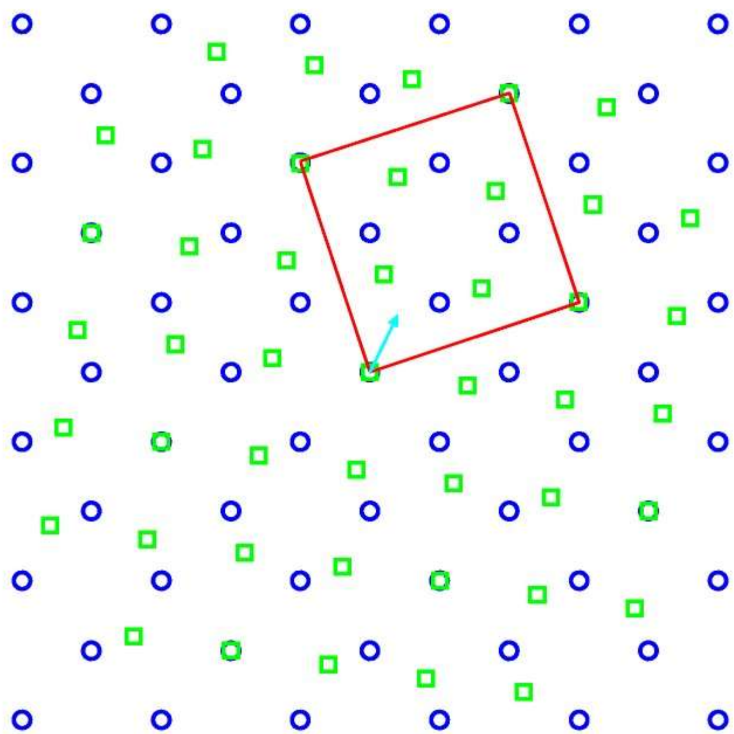
First principles DENSITY FUNCTIONAL THEORY simulations (→ accurate description of the interatomic bonding)

SELECTED GRAIN BOUNDARIES

Σ=5 (001) TWIST

rotational axis perpendicular to boundary plane



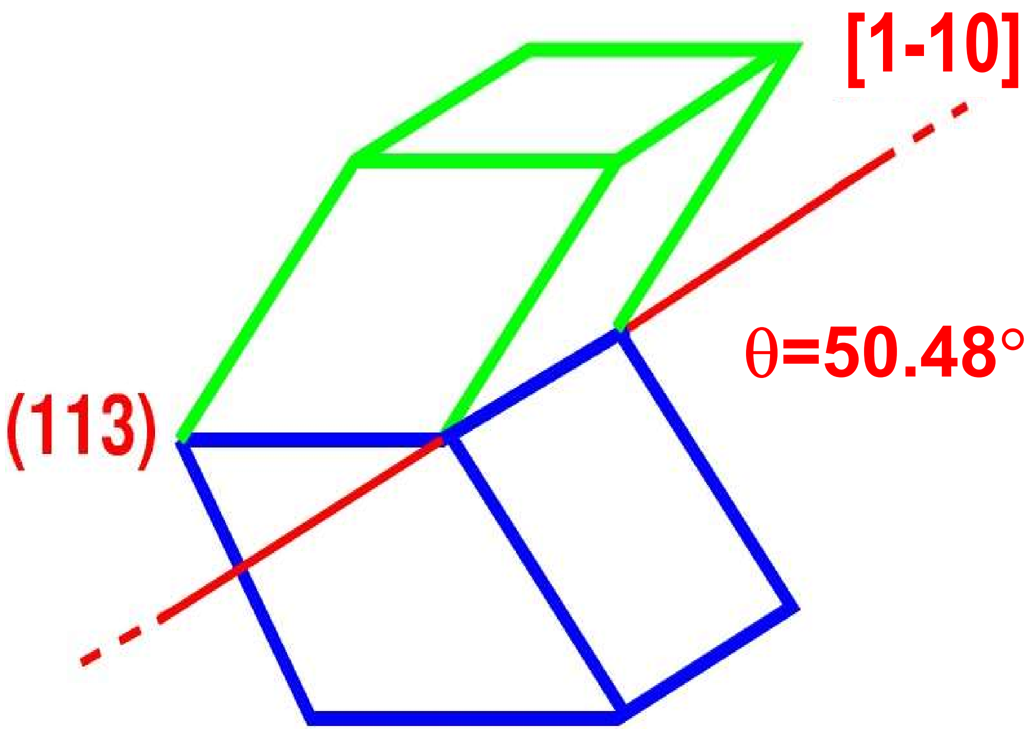


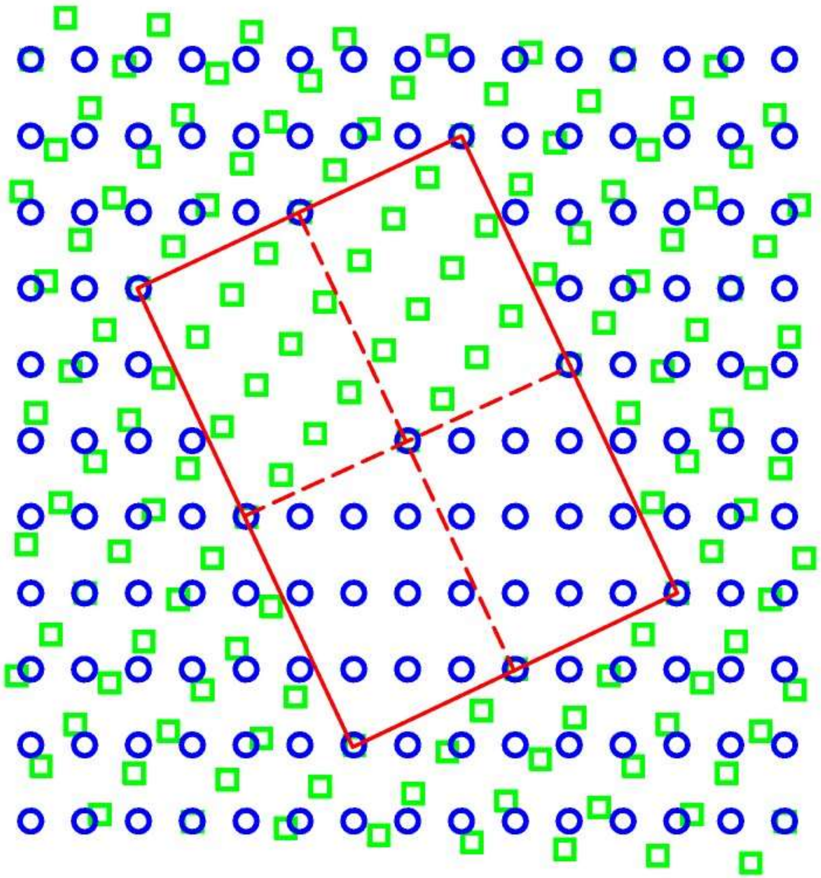
COINCIDENCE SITE LATTICE
[CSL]

SELECTED GRAIN BOUNDARIES

Σ=11 (113), 50.48°[1-10] TILT

rotational axis parallel to boundary plane





BOUNDARIES AND MATERIALS

- **GERMANIUM (brittle semiconductor)**

  Σ=5 (001) TWIST BOUNDARY

  C.Molteni, G.P. Francis, M.C. Payne and V. Heine, Phys. Rev. Lett. 76, 1284 (1996)

  [reviewed in T. Arias, "Theorist Learn to Slip and Slide", Physics World 9, 22 (1996)]

  C. Molteni, G.P. Francis, M.C. Payne and V. Heine, Materials Science and Engineering B 37, 121 (1996)

- **ALUMINIUM (ductile metal)**

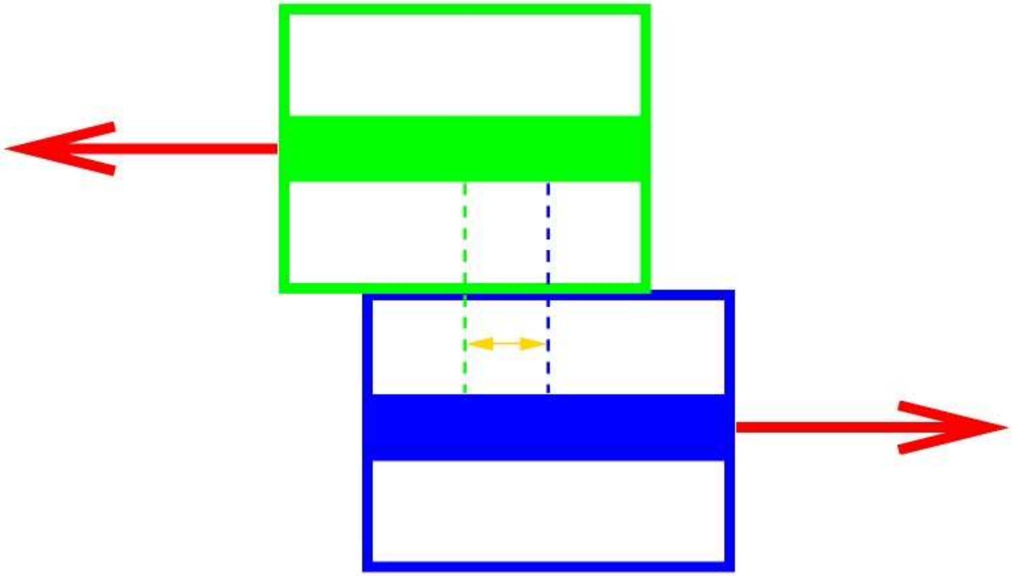
  Σ=5 (001) TWIST BOUNDARY

  Σ=11 (113), 50.48 [1-10] TILT BOUNDARY

  C. Molteni, N. Marzari, M.C. Payne and V. Heine, Phys. Rev. Lett. 79, 869 (1997)

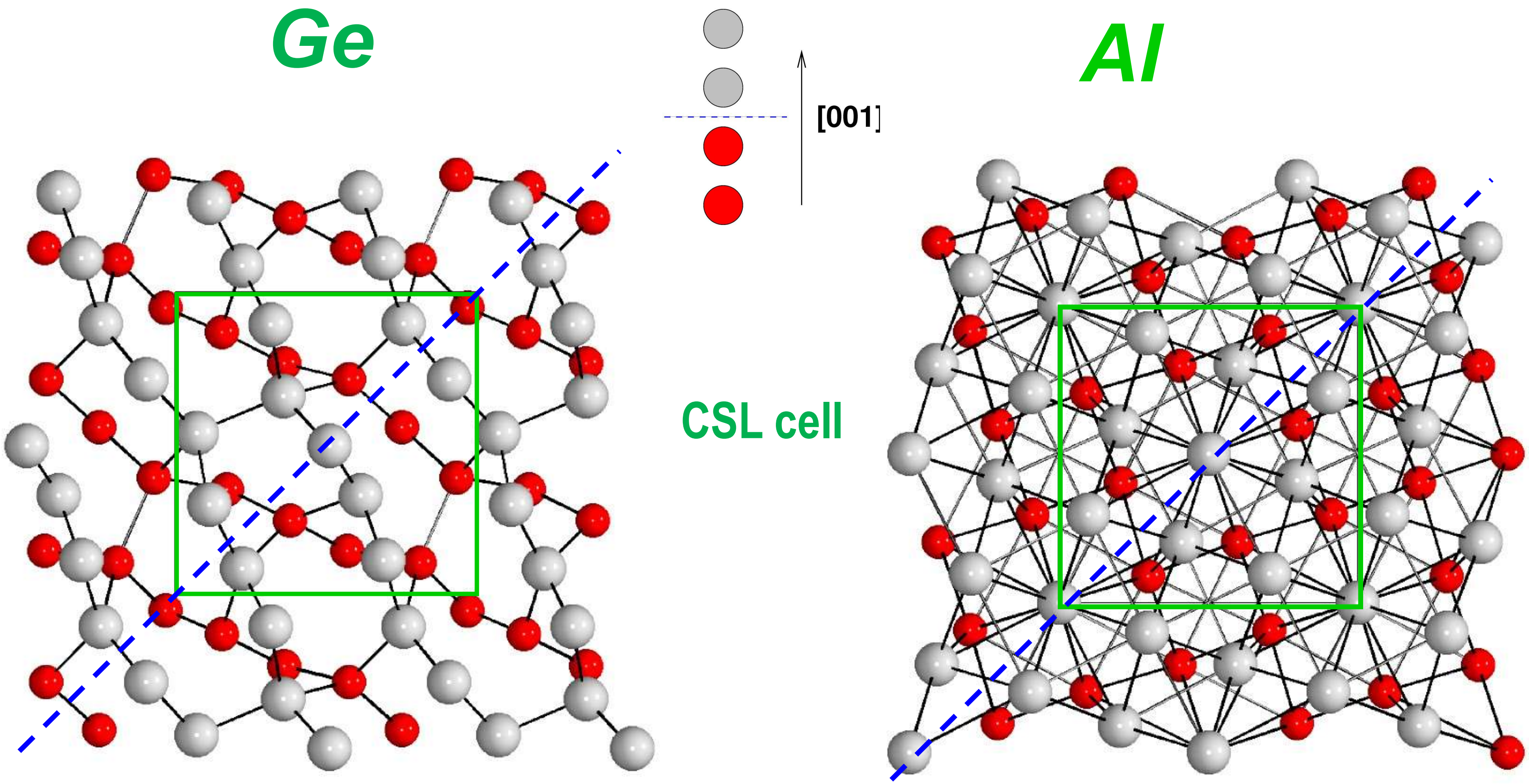
  C. Molteni, "Modelling grain boundary sliding from first principles", Mater. Sci. Forum 447-448, 11-17 (2003)

MODELLING THE SLIDING PROCESS



- **Quasi-static simulation**
  - Constant strain increment & structural relaxations at each step
- **Total energy calculations DFT-LDA, pseudopotentials, plane-waves (CASTEP)**
  - Ensemble DFT for metals (*N. Marzari et al., Phys. Rev. Lett. 79, 1337 (1997)*)
- **Supercells** (two equivalent grain boundaries)
  - Ge twist: 70 atoms (14 layers); Al twist: 60 atoms (12 layers)
  - Al tilt: 44 atoms (22 layers)

Σ=5 (001) TWIST GRAIN BOUNDARIES



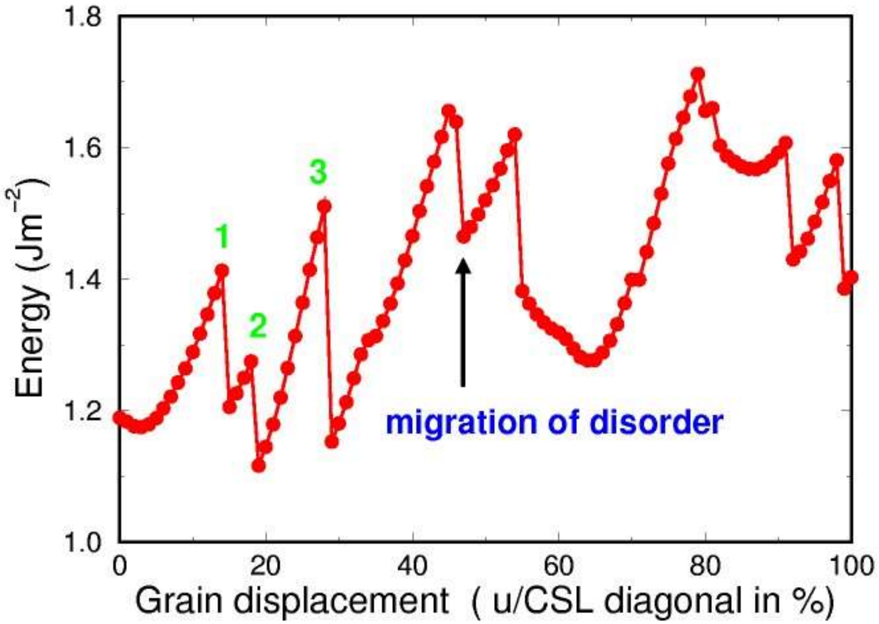
Sliding direction
[120]

Translational state (-1/20;1/20)

Translational state (0;0)

Σ=5 (001) TWIST BOUNDARY in Ge

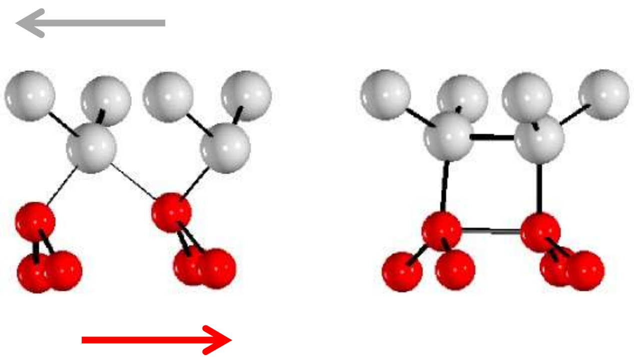
Stick-slip mechanism



Rebonding events

1st energy jump

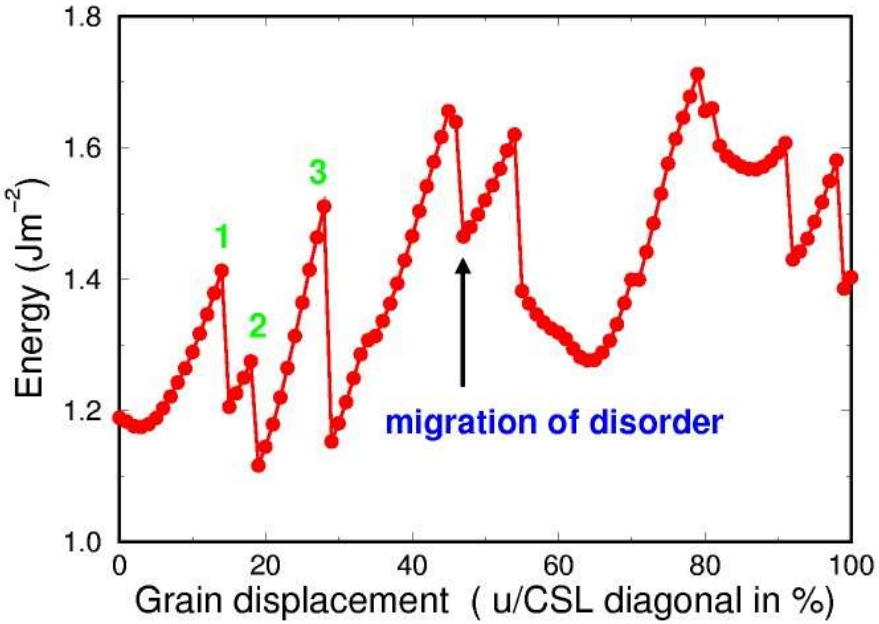
before



after

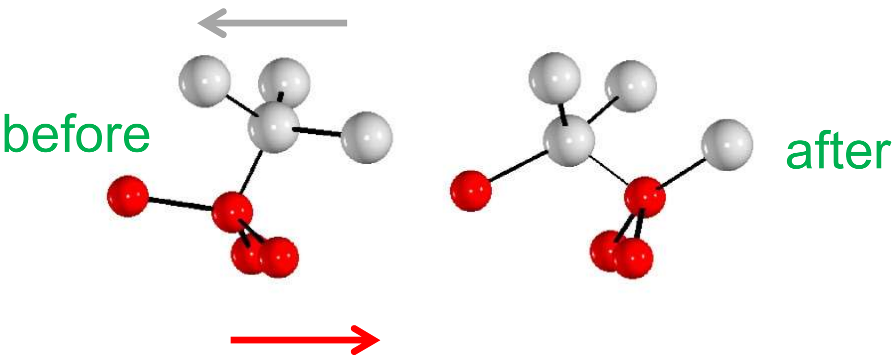
Σ=5 (001) TWIST BOUNDARY in Ge

Stick-slip mechanism



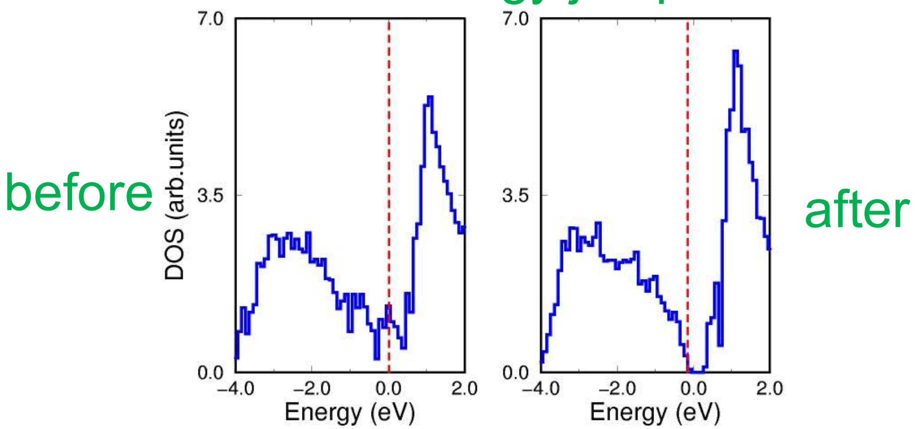
Rebonding events

2nd energy jump



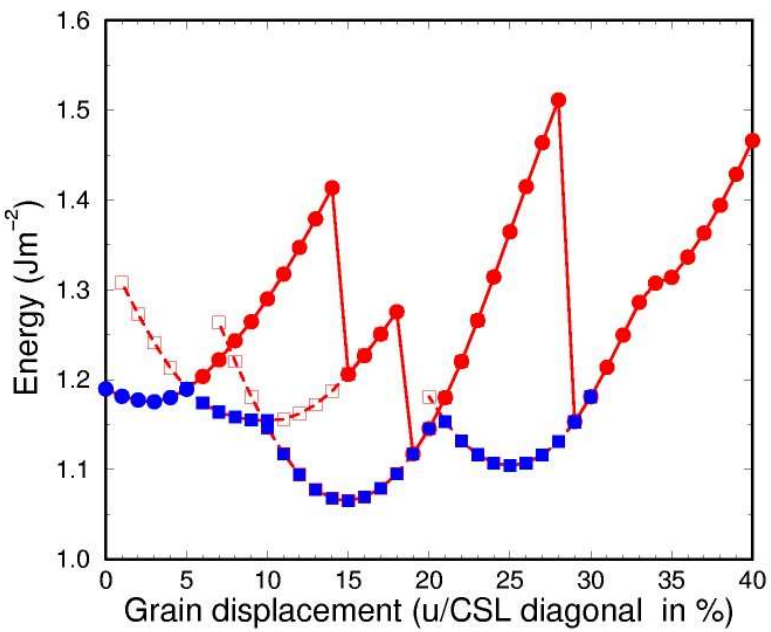
Clearing of gap states

3rd energy jump

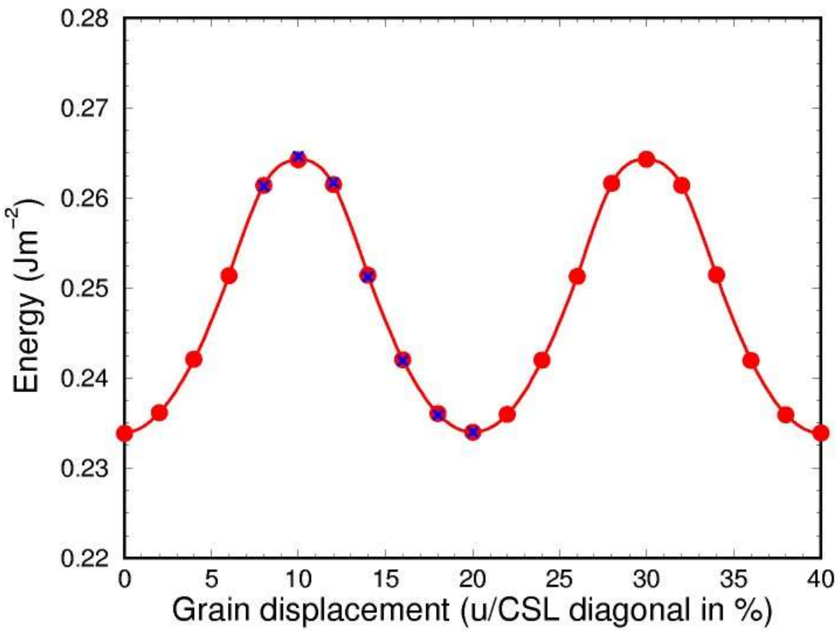


Σ=5 (001) TWIST BOUNDARIES

Ge



Al

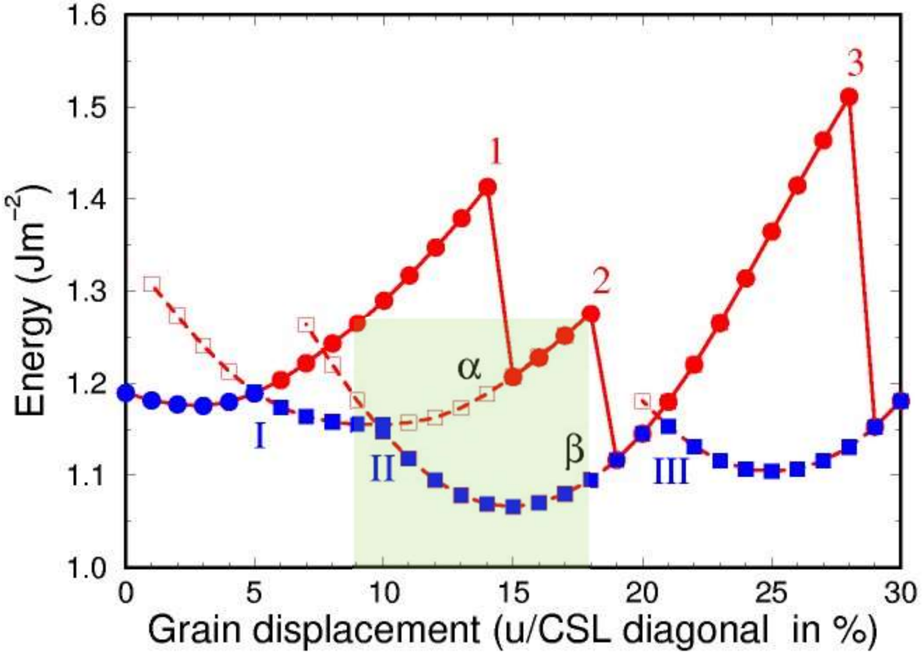


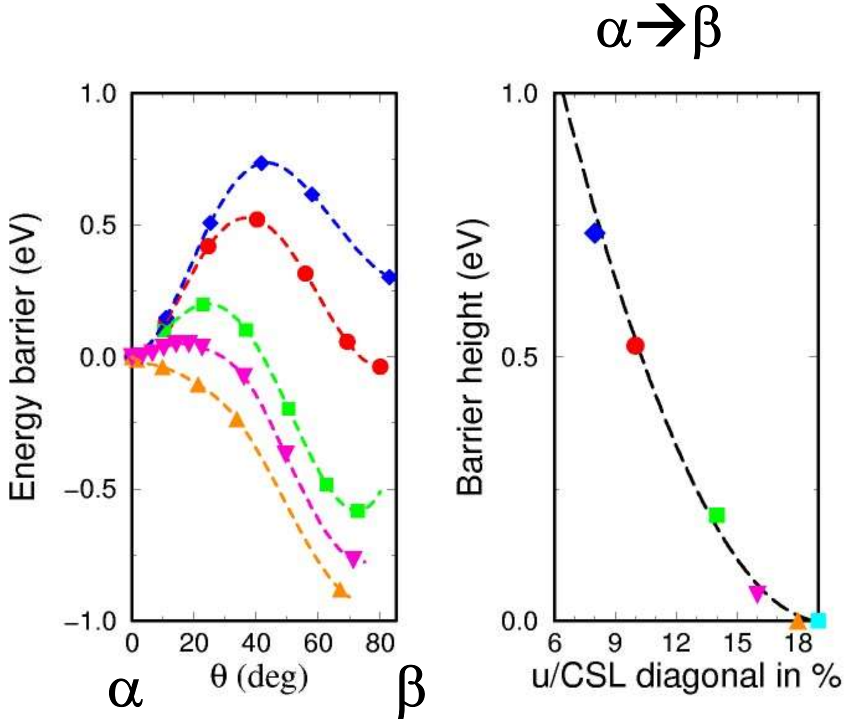
Forward sliding

Backward sliding

TEMPERATURE AND STRAIN RATE EFFECTS

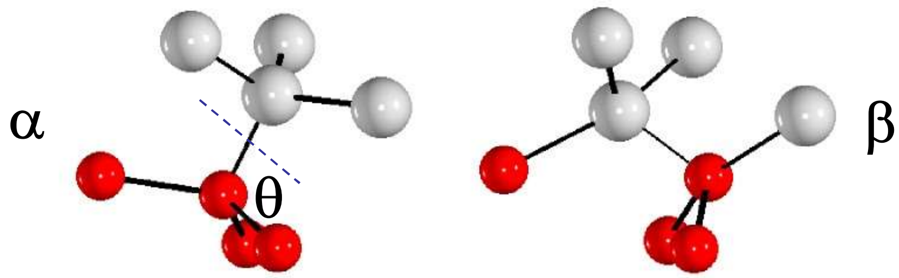
Σ=5 (001) twist boundary in Ge





low T, high v

high T, low v



TEMPERATURE AND STRAIN RATE EFFECTS

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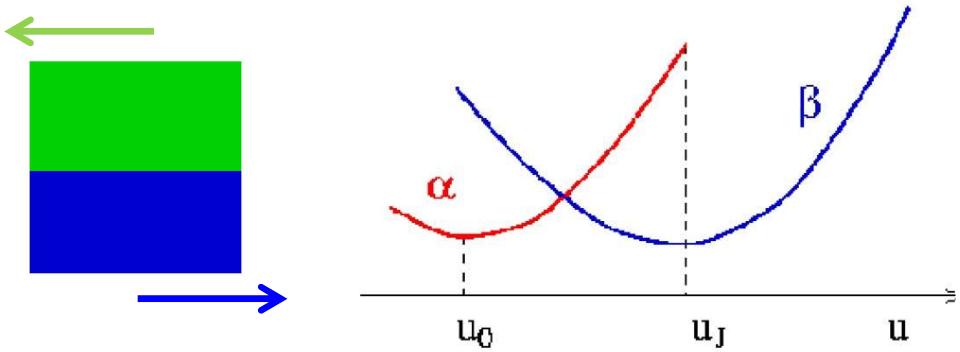
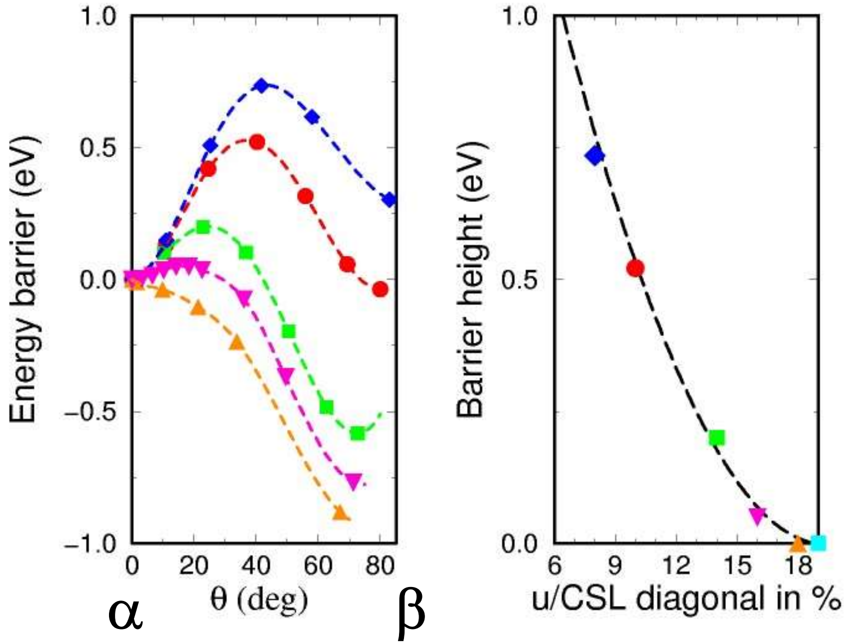




$u=u_0+vt \quad v=\mathrm{const}$

$$\kappa^{\alpha\beta}=\nu\exp\left[{-E_b^{\alpha\beta}(u)}\big/{K_BT}\right]$$

$$\kappa^{\beta\alpha}=\nu\exp\left[{-E_b^{\beta\alpha}(u)}\big/{K_BT}\right]$$

$$\begin{cases}\dot P_\alpha=-\kappa^{\alpha\beta}P_\alpha+\kappa^{\beta\alpha}P_\beta\\ \dot P_\beta=+\kappa^{\alpha\beta}P_\alpha-\kappa^{\beta\alpha}P_\beta\end{cases}$$

$t_R \Leftrightarrow P_\beta(t_R)=1/2$

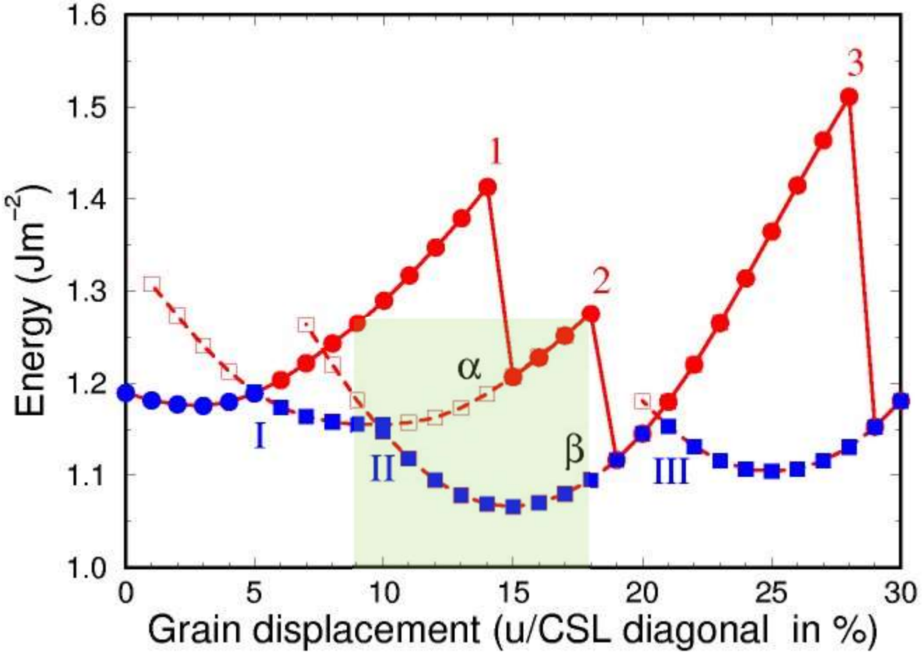
$u_R=u_0+vt_R$

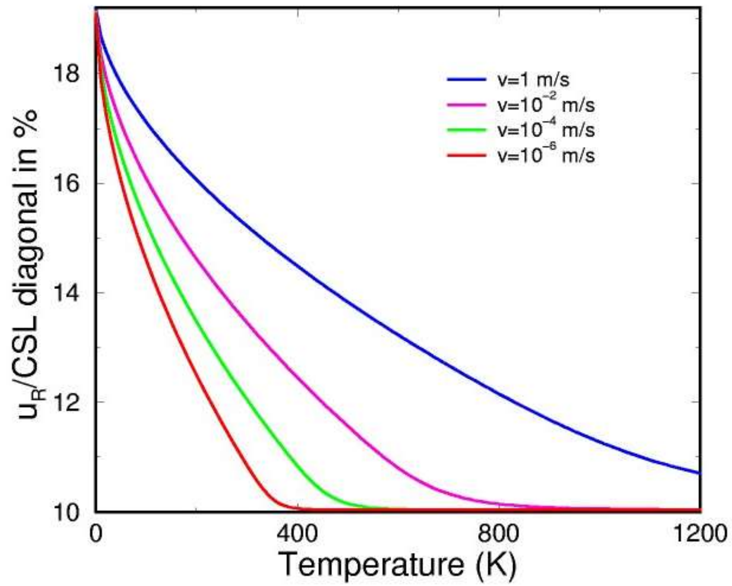
$$\sigma=\frac{1}{u_J-u_0}\int_{u_0}^{u_J}\left[\sigma_\alpha P_\alpha du+\sigma_\beta P_\beta du\right]$$

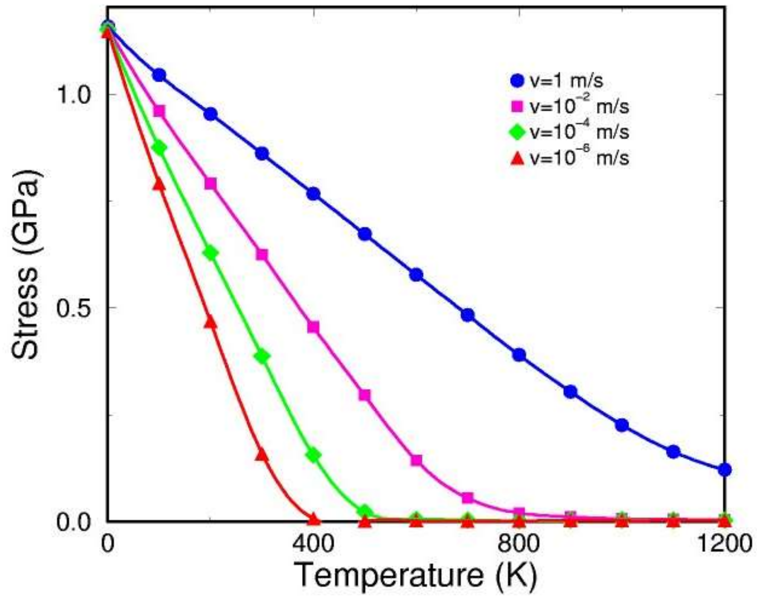
$$\Delta\sigma=\sigma-\sigma_{highT}$$

TEMPERATURE AND STRAIN RATE EFFECTS

Σ=5 (001) twist boundary in Ge

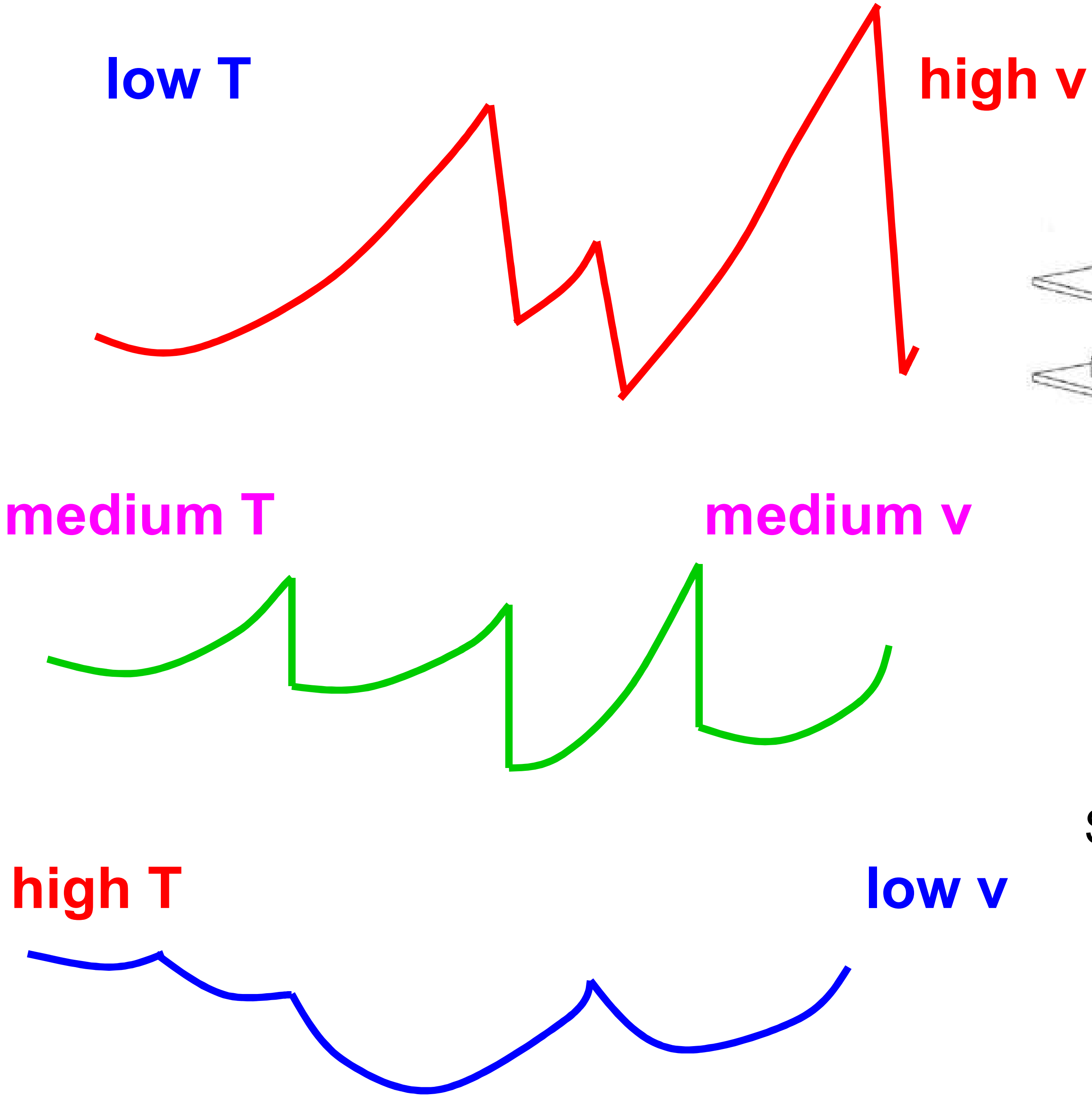


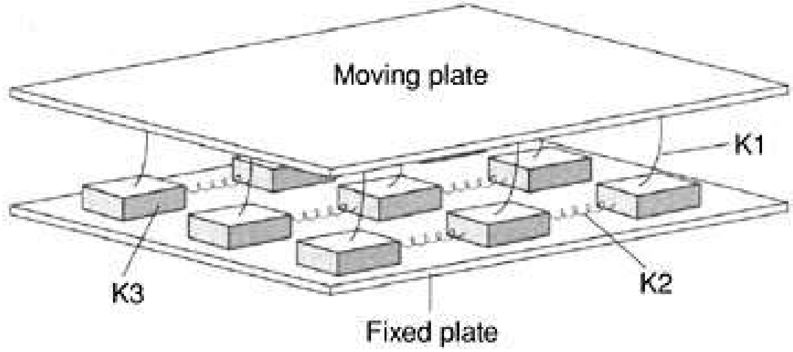




low T, high v **high T, low v**

TEMPERATURE AND STRAIN RATE EFFECTS



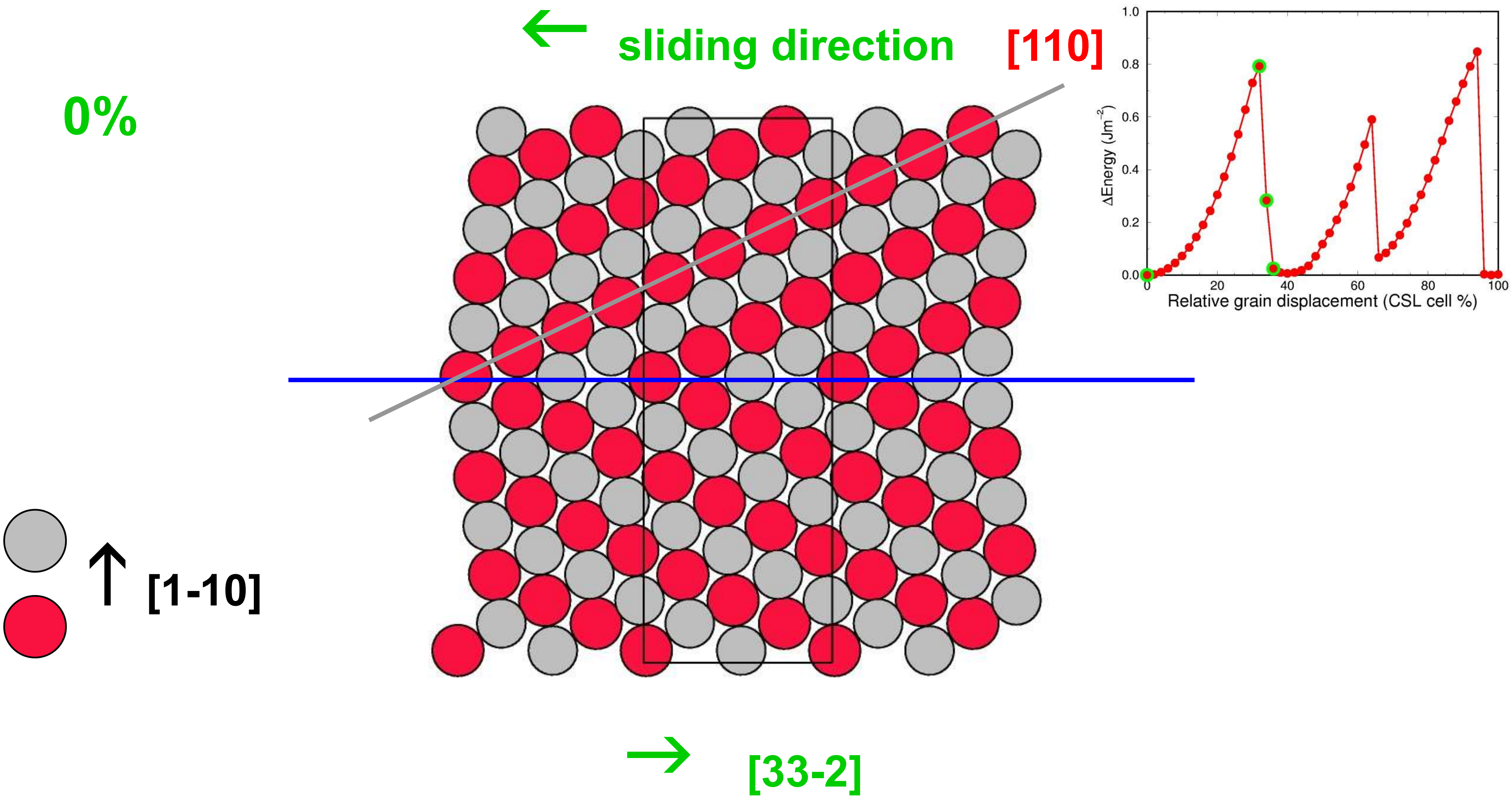


https://www.nap.edu/

spring-block
earthquake model

Self-organized criticality?

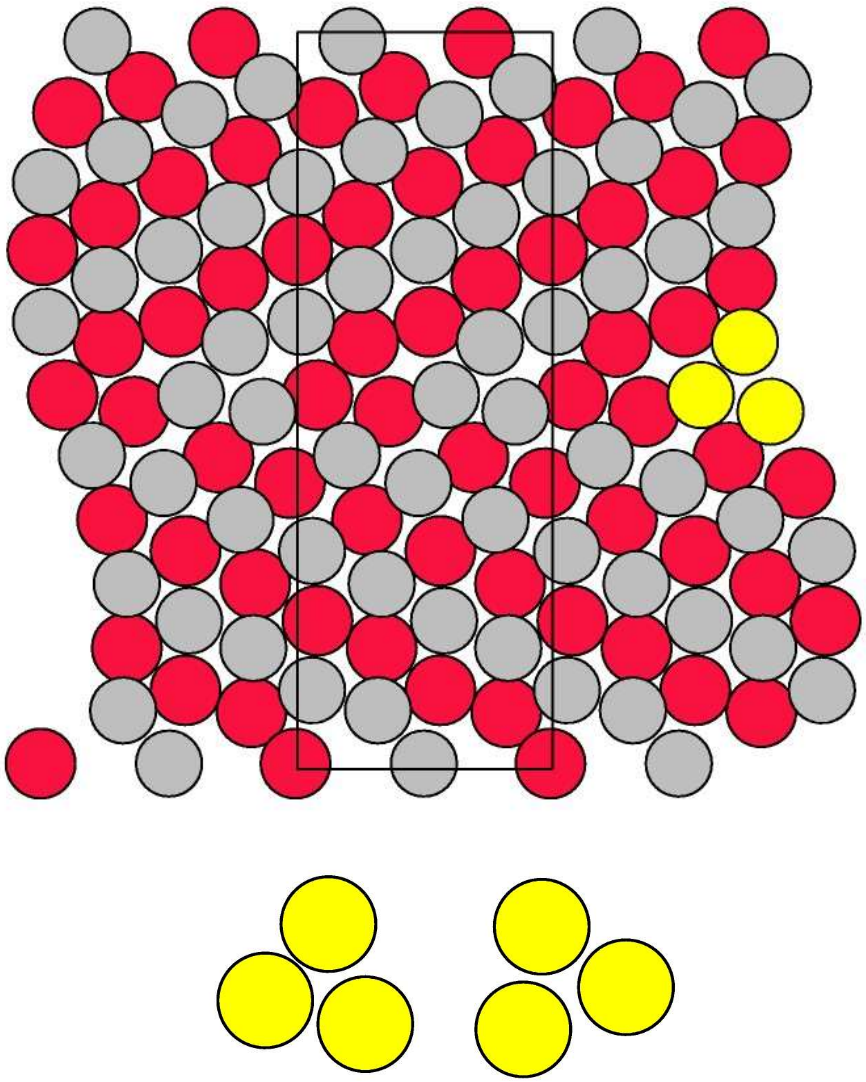
SLIDING-INDUCED MIGRATION

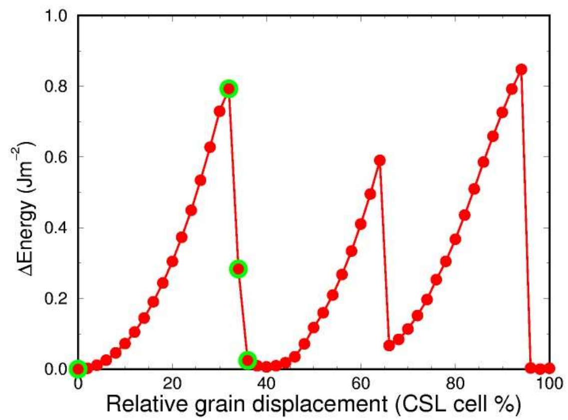


Al Σ=11 (113), 50.48° [1-10] TILT BOUNDARY

SLIDING-INDUCED MIGRATION

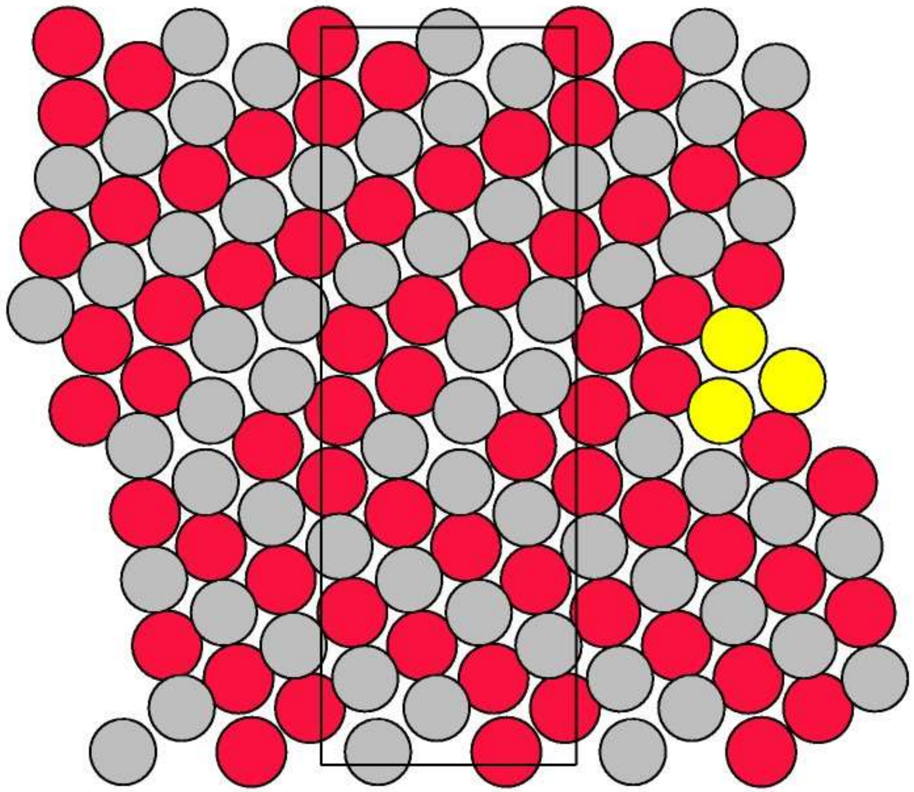
32%

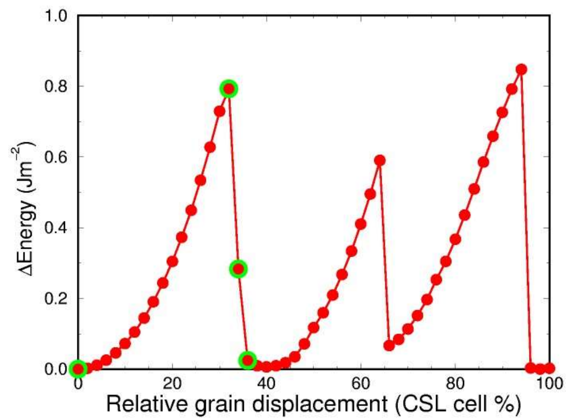


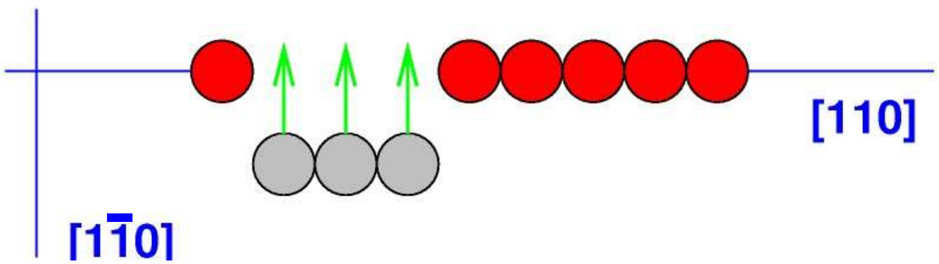


SLIDING-INDUCED MIGRATION

34%

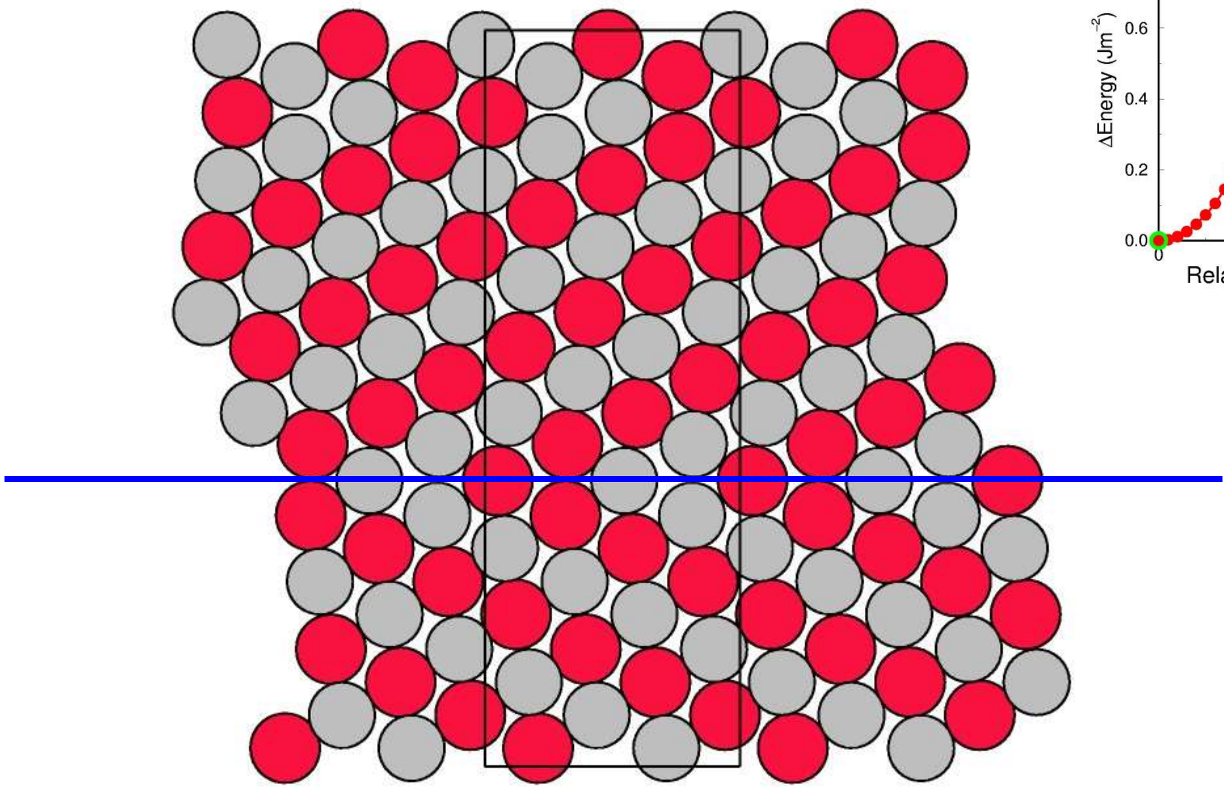


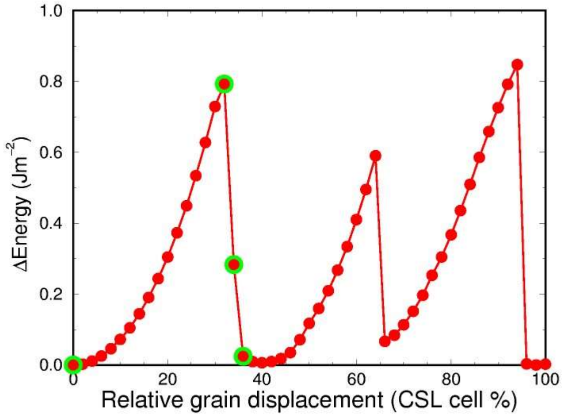




SLIDING-INDUCED MIGRATION

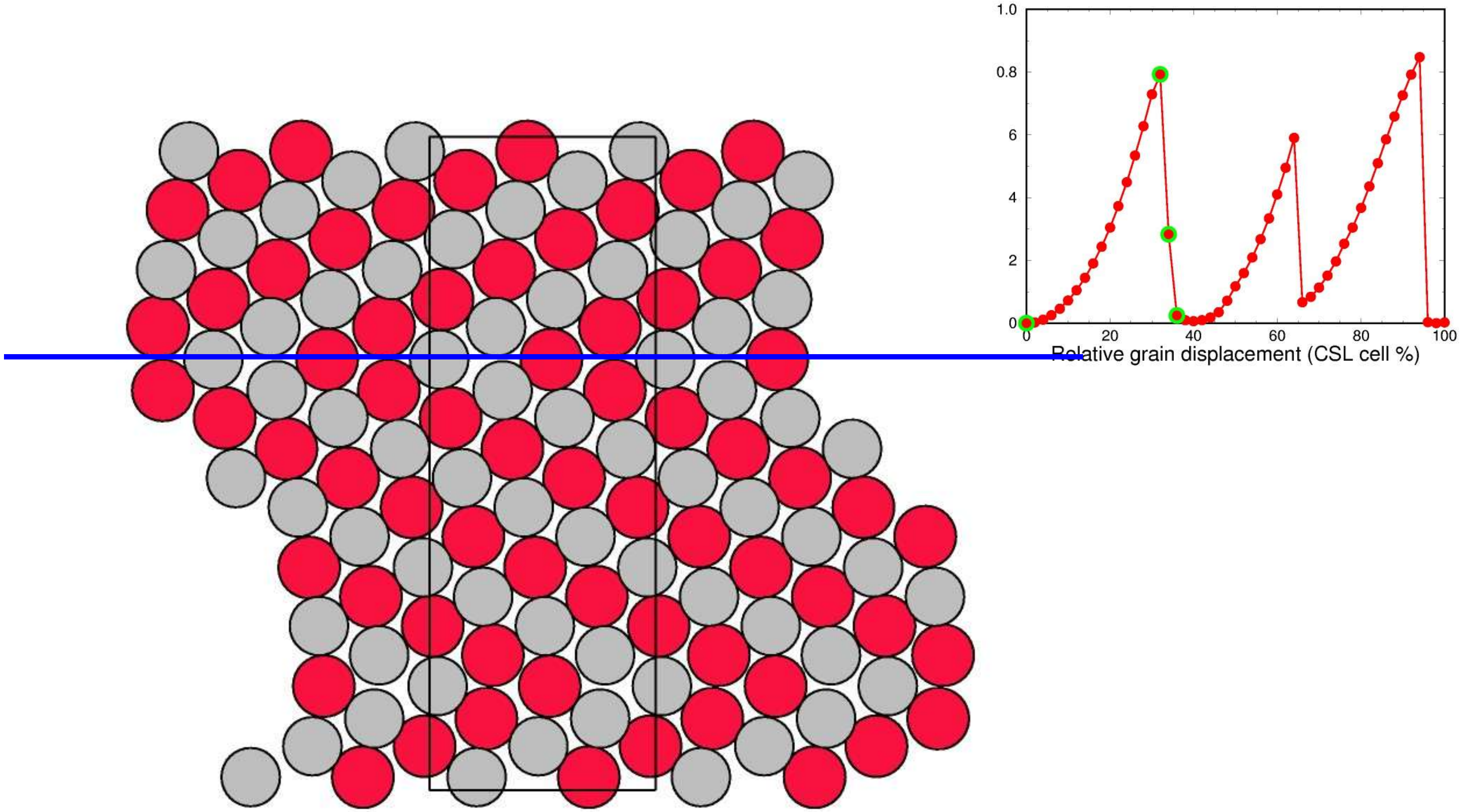
36%





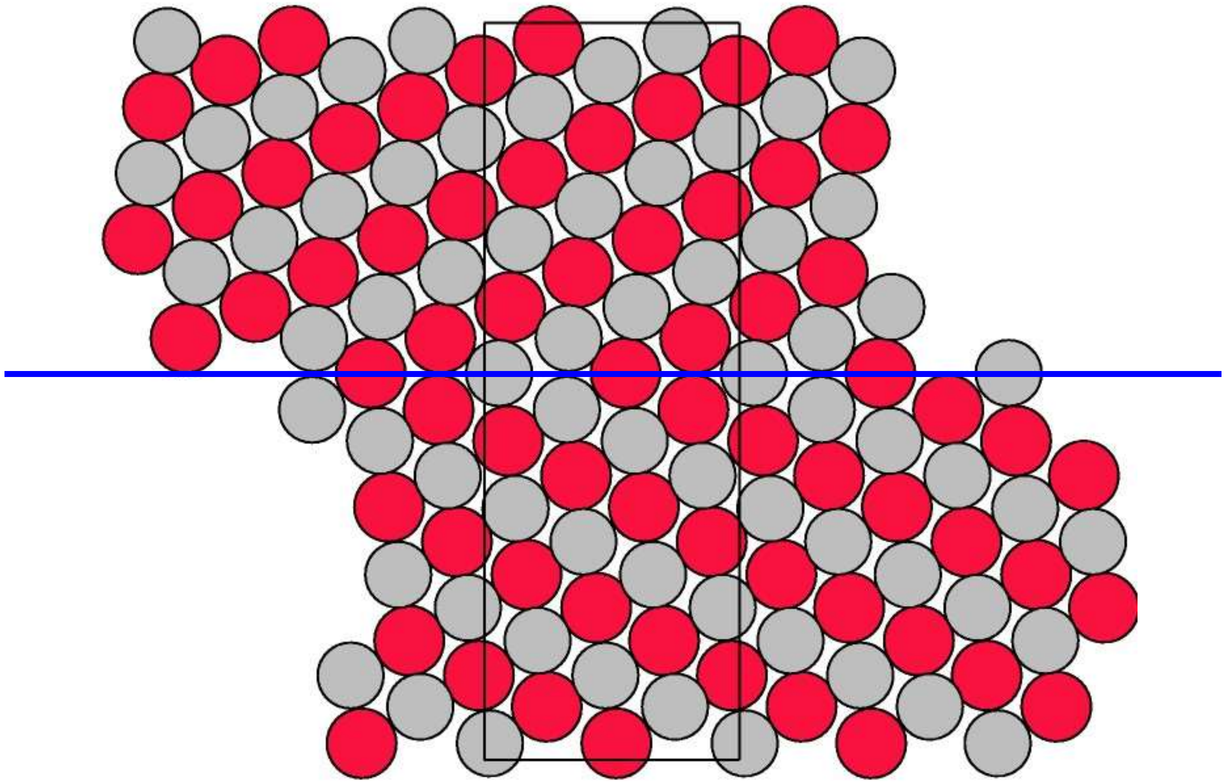
SLIDING-INDUCED MIGRATION

66%



SLIDING-INDUCED MIGRATION

96%



CONCLUSIONS

- A variety of sliding behaviours, that depend not only on the material, but also on the boundary geometry, the local order and the presence of defects, have been found.

- While sliding in Ge is controlled by local stick-slip events involving rebonding of a few atoms at the boundary interface, in Al a larger number of atoms act in concert over extended areas, ultimately limited by boundary defects.

- Still to be done: Ga in Al grain boundaries, sliding in ice grain boundaries, the quake model…

Acknowledgements

- Mike C. Payne & Volker Heine (Cambridge University)
- Nicola Marzari (EPFL)
- Graeme P. Francis (?)
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- All TCM
- EC – Human Capital & Mobility programme