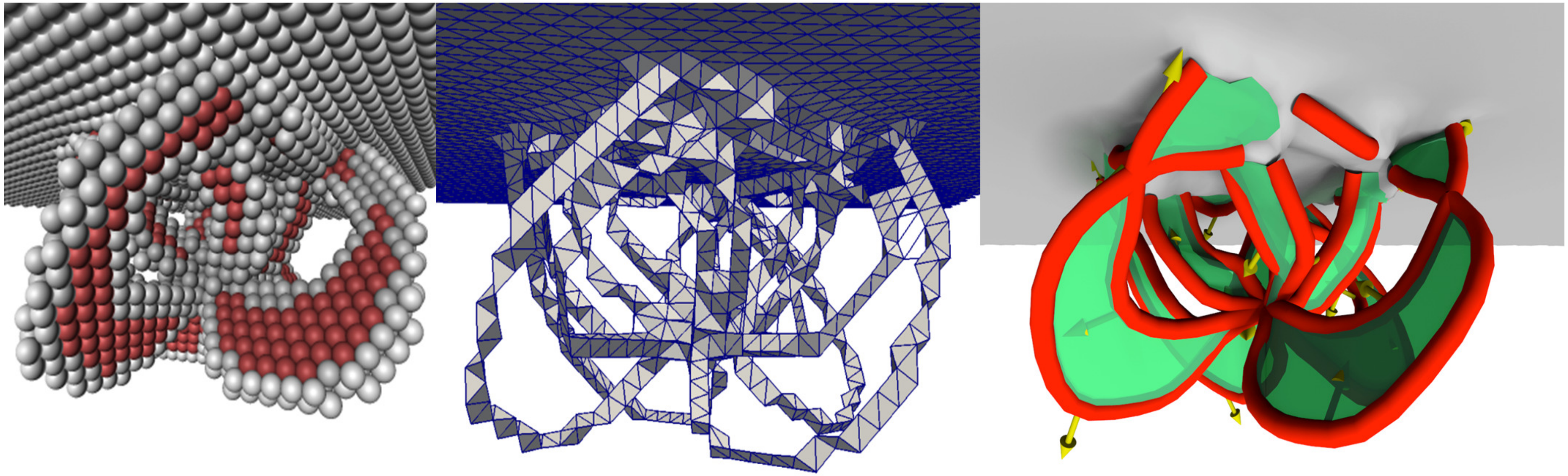
Deformation behaviour of nanocrystalline metal alloys simulated by *hybrid MD/MC simulations*

<u>Karsten Albe</u>, Jonathan Schäfer, Alexander Stukowski, Yvonne Ritter

TU Darmstadt. Institut für Materialwissenschaft, FG Materialmodellierung
Funded by DFG „Forschergruppe 714"



Plastic deformation

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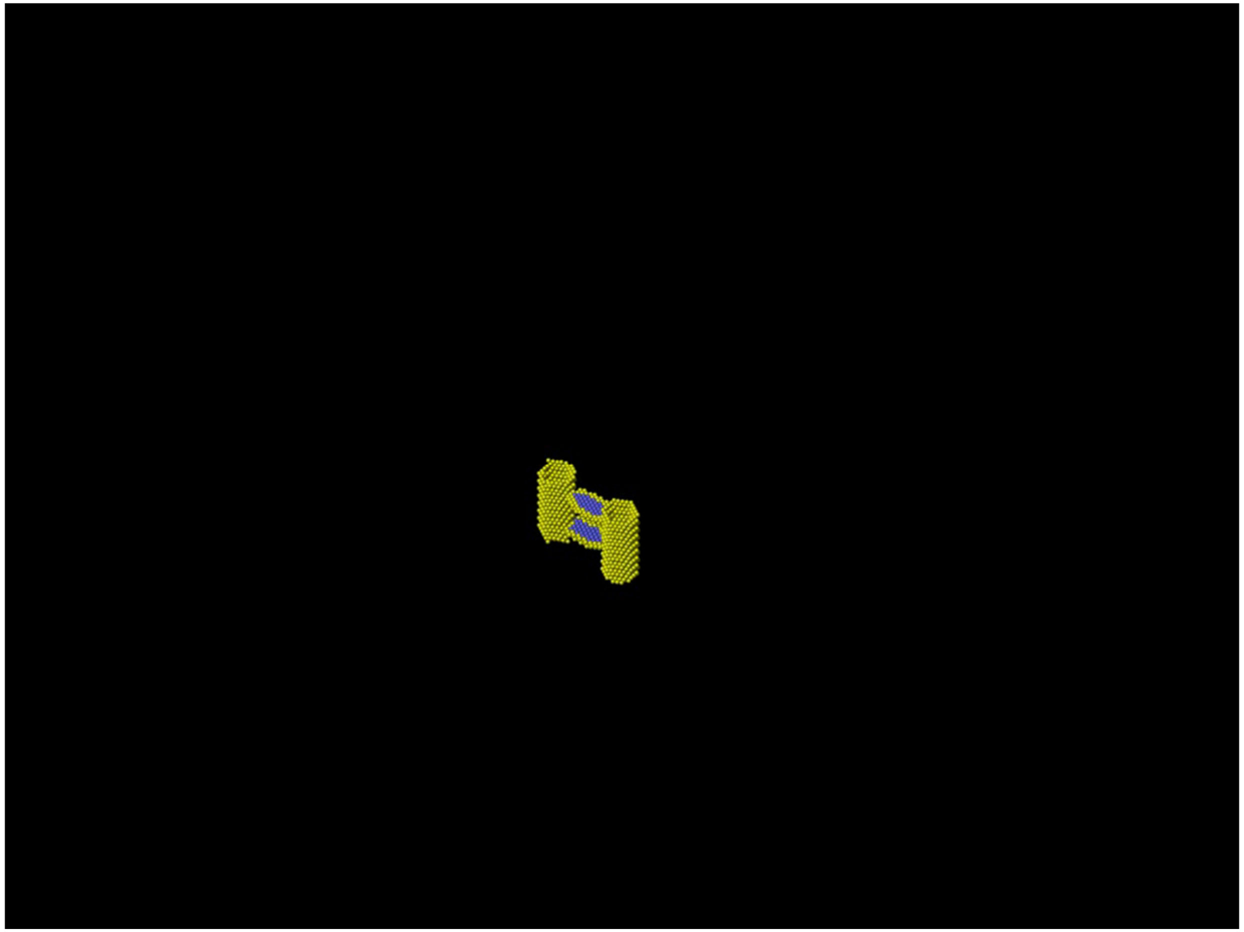

Strengthening metals and alloys

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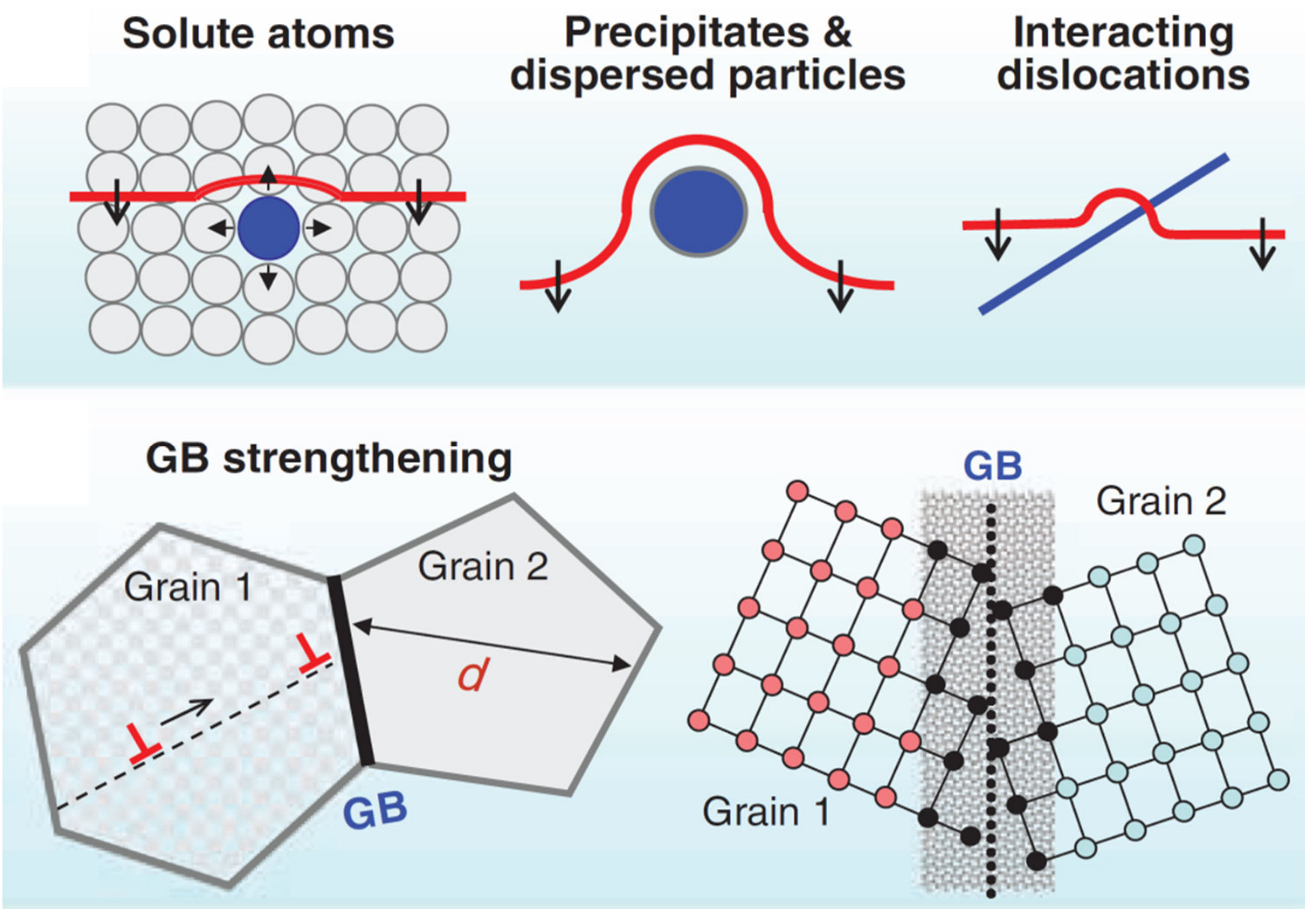

Nanocrystalline metals

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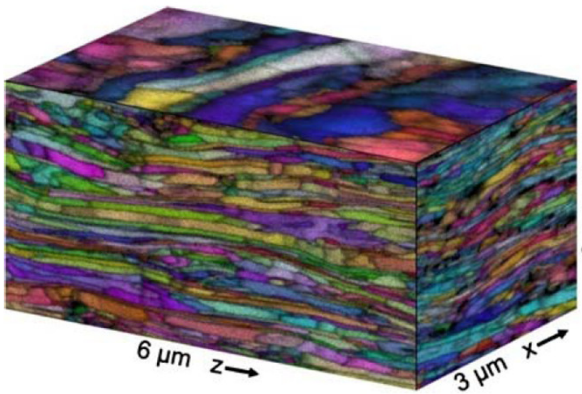
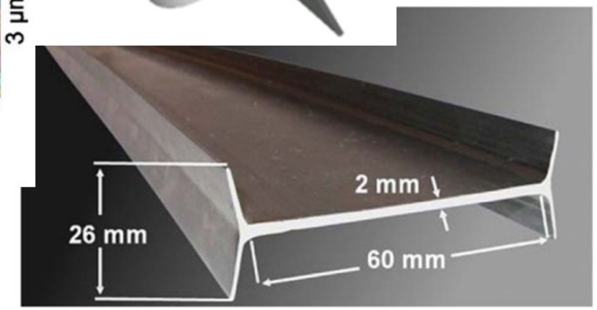
Microstructure

- Grain size D < 100 nm
- Large fraction of grain boundaries

Special properties

- Increased strength
- High wear resistance
- Superplasticity

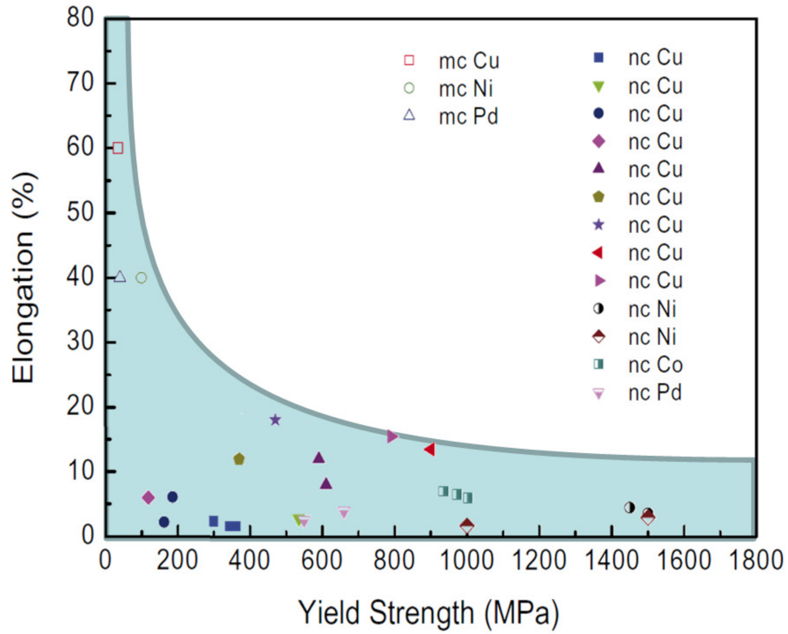




Linear Flow Splitting

Bohn et al., J Mater Sci 43 (2008) 7307

Ductility ⟷ Strength



Dao et al., Acta Mater 55 (2007) 4041

nc-Metals: Insights and Puzzles

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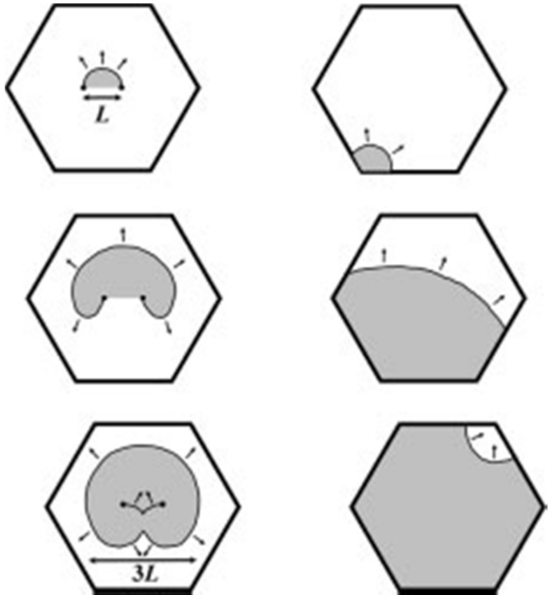
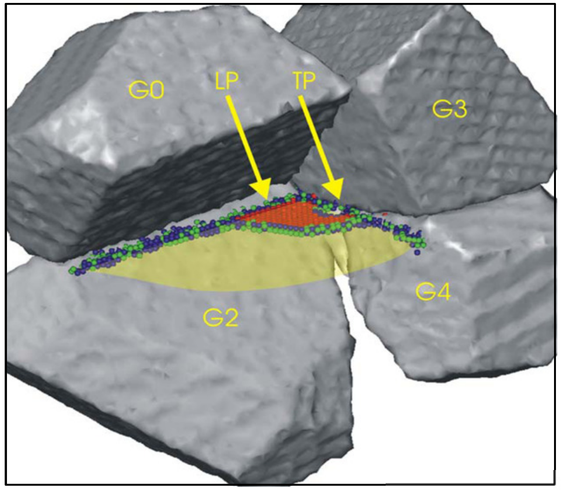
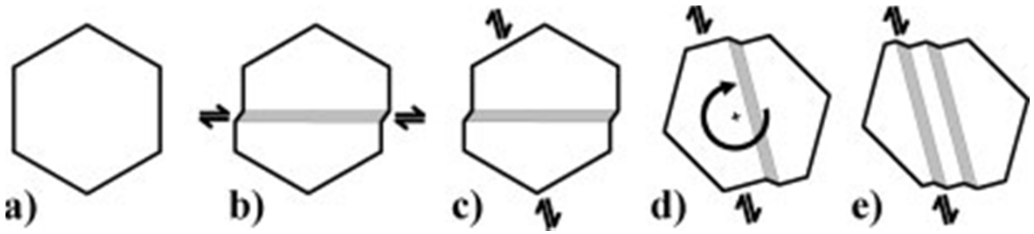
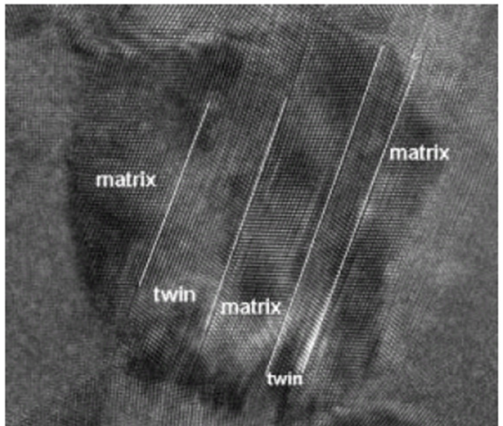




Van Swygenhoven et al., Acta Mat., 54 (2006)

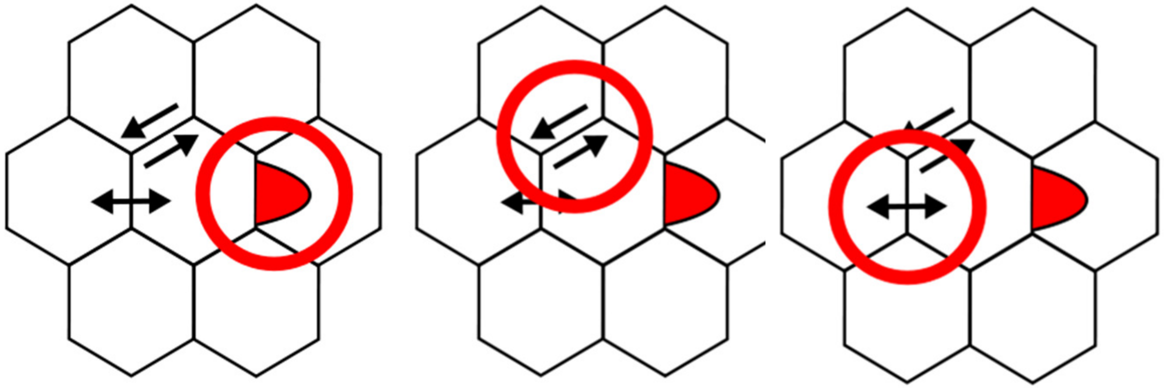


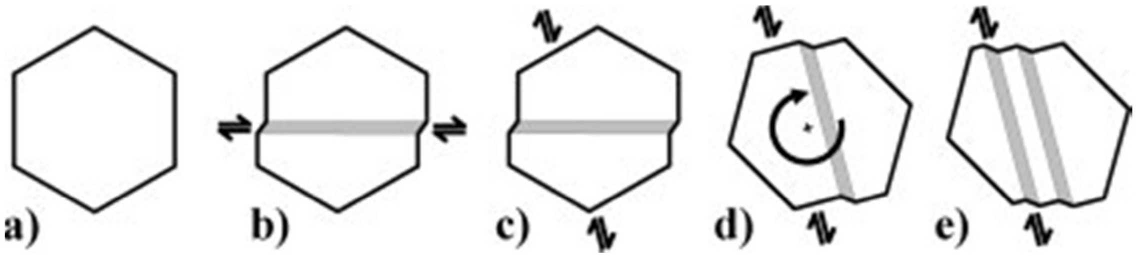
ADVANCED ENGINEERING MATERIALS **2005**, *7*, No. 4

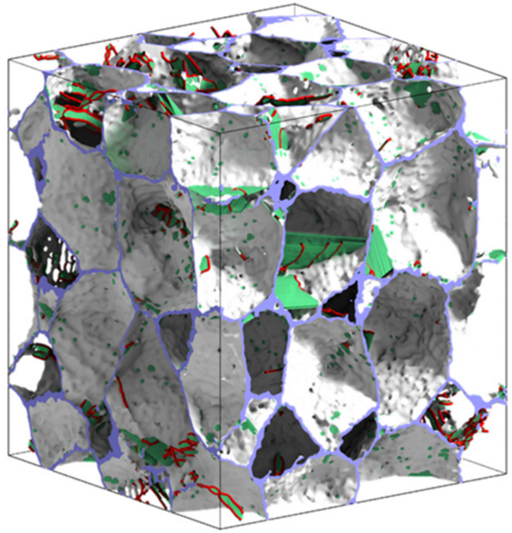


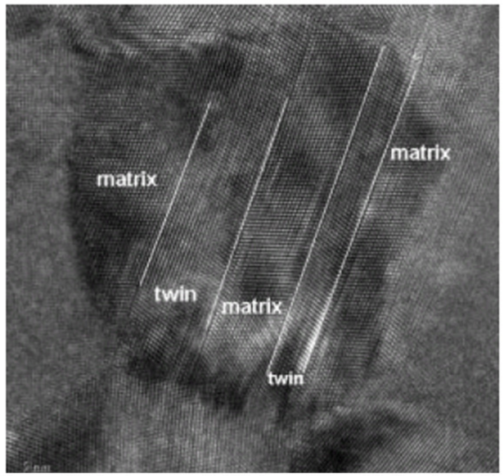
H. Rösner, J. Markmann, J. Weissmüller, *Philos. Mag. Lett.* **2004**, *84*, 321.

nc-Metals: Insights and Puzzles



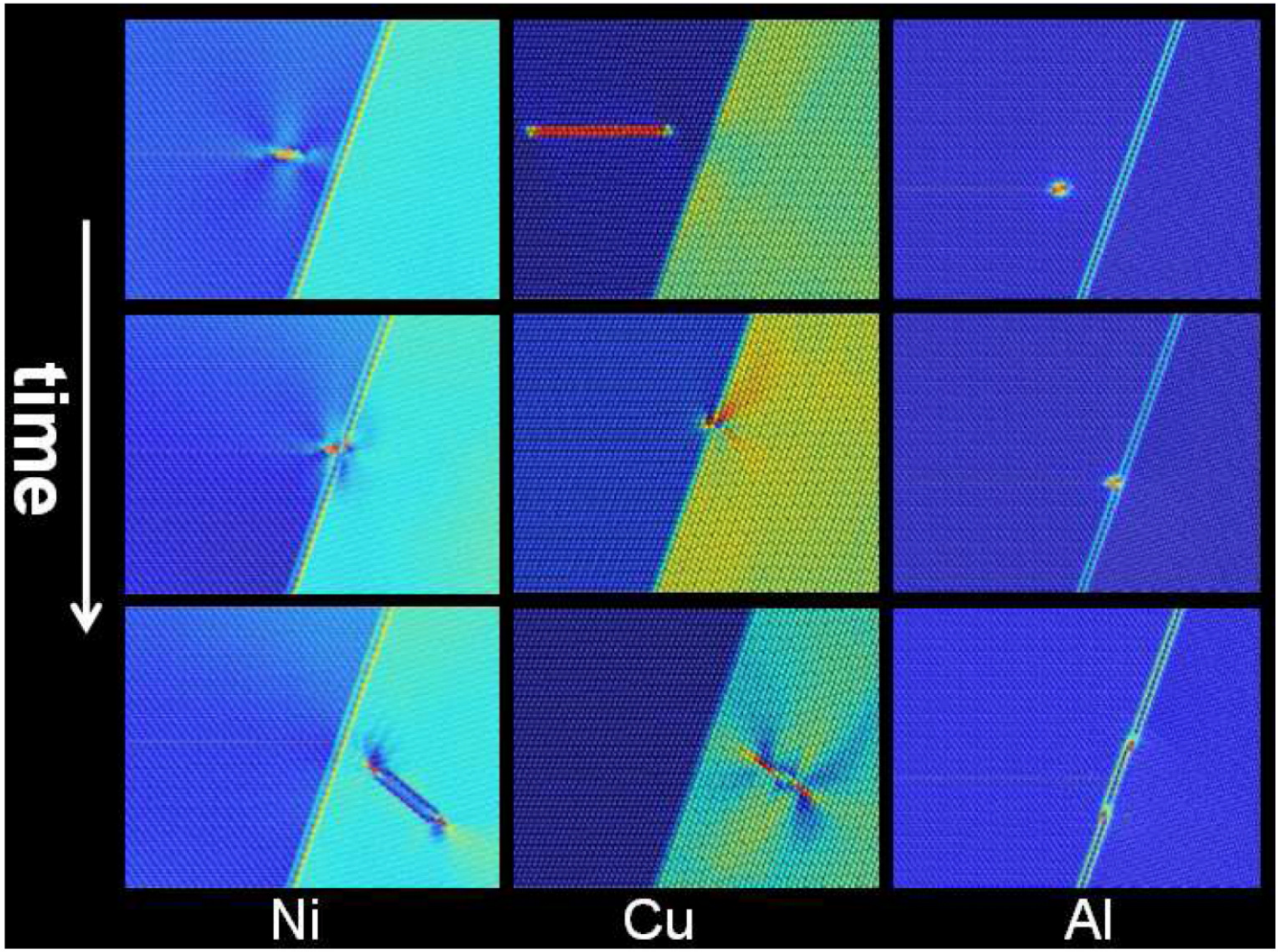






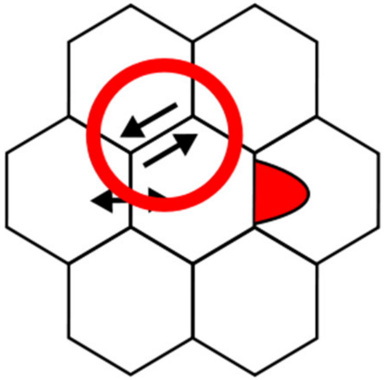
H. Rösner, J. Markmann, J. Weissmüller, *Philos. Mag. Lett.* **2004**, *84*, 321.

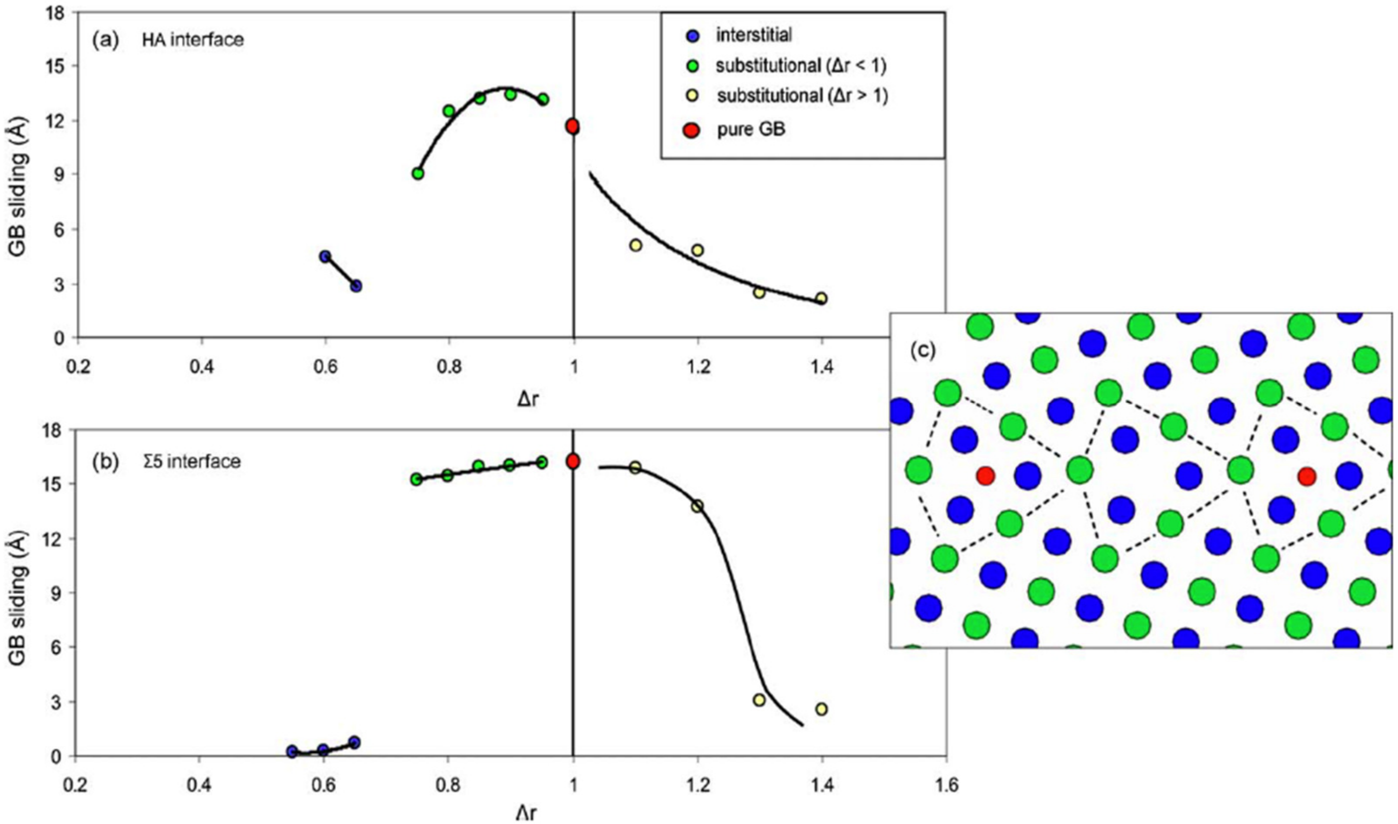
Example: Dislocation-Twin Interaction



ZH Jin, K. Albe et al. Scripta Materialia 54 (6), 1163-1168

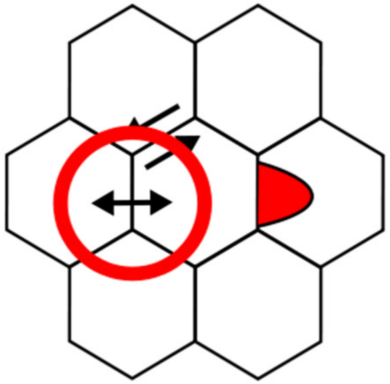
GB sliding

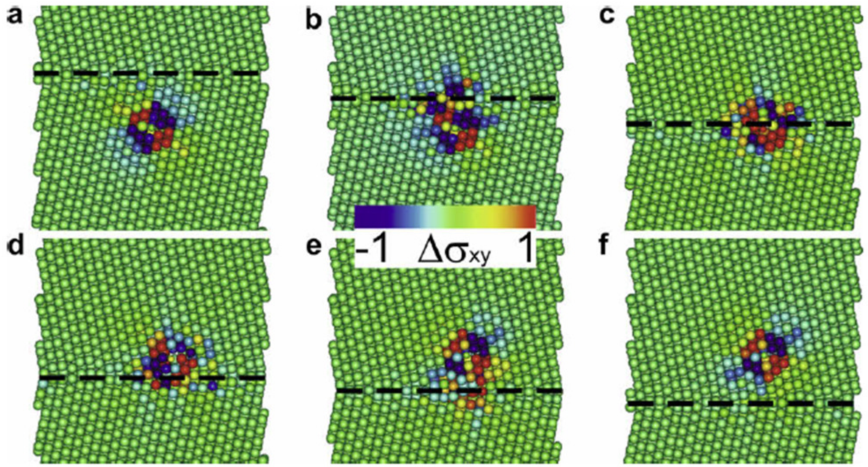


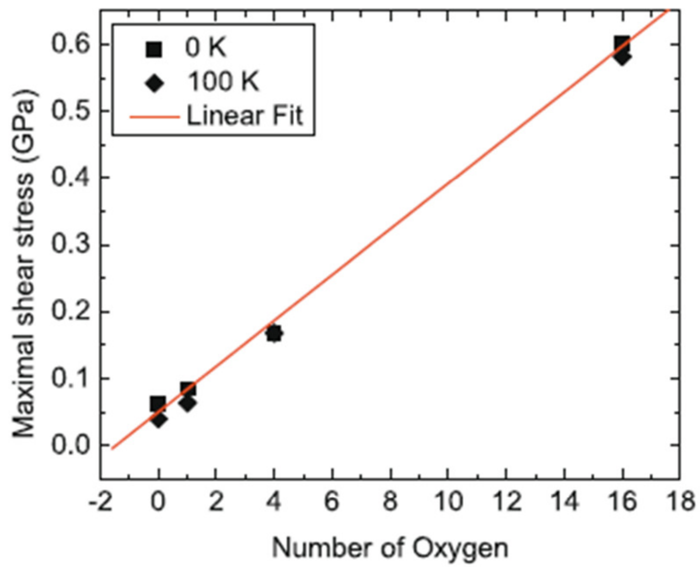


Millett et al., Mat. Sci. Eng. A, 431 (2006)

Coupled GB motion

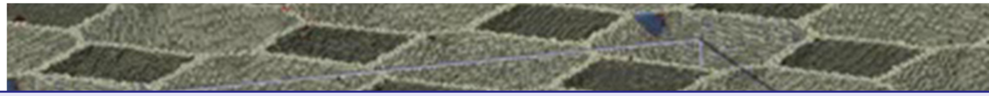






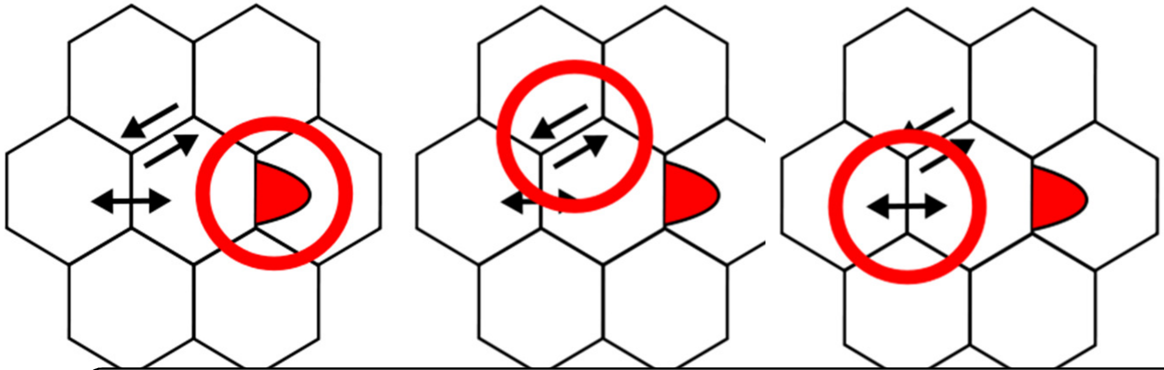
Elsener et al., Acta Mater., 57 (2009)

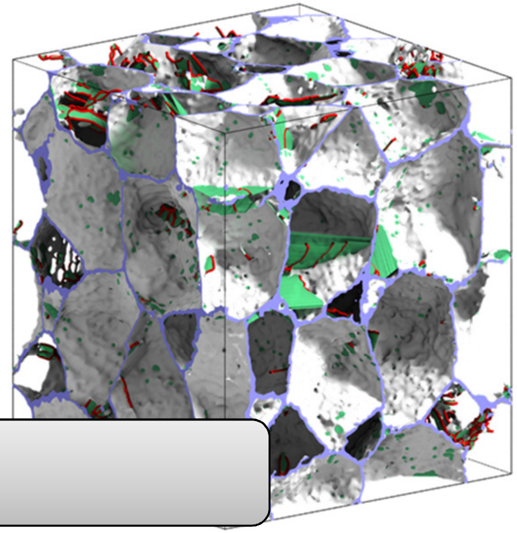
MD-Simulations of nc-metals



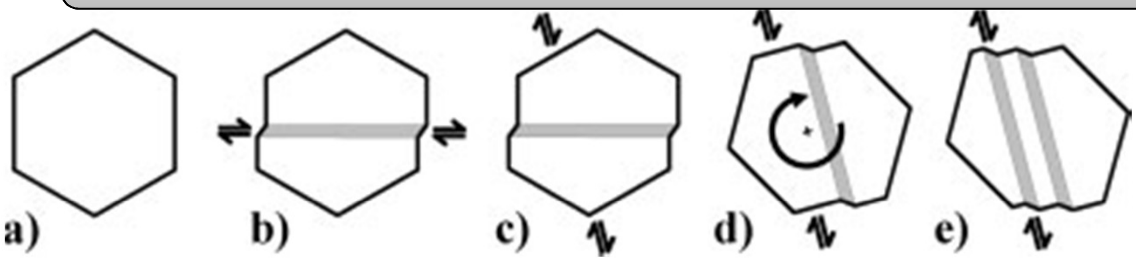
- Realistic interatomic potentials?
- How to get realistic virtual structures?
- How do we deal with the presence of solutes?
- How to analyse the data and transfer information from atomistic into continuum models?
- How to get to realistic strain rates?

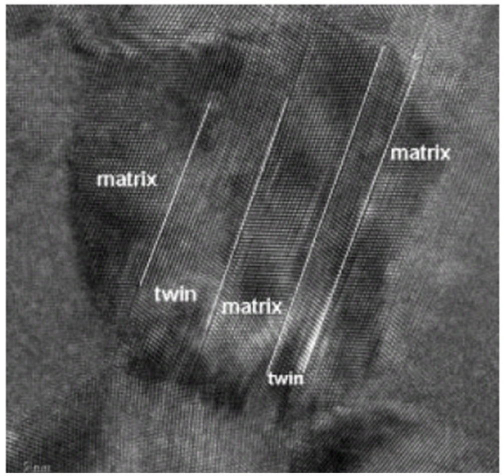
nc-Metals: Insights and Puzzles





Influence of solutes ?





H. Rösner, J. Markmann, J. Weissmüller, *Philos. Mag. Lett.* **2004**, *84*, 321.

nc-Metals: Insights and Puzzles

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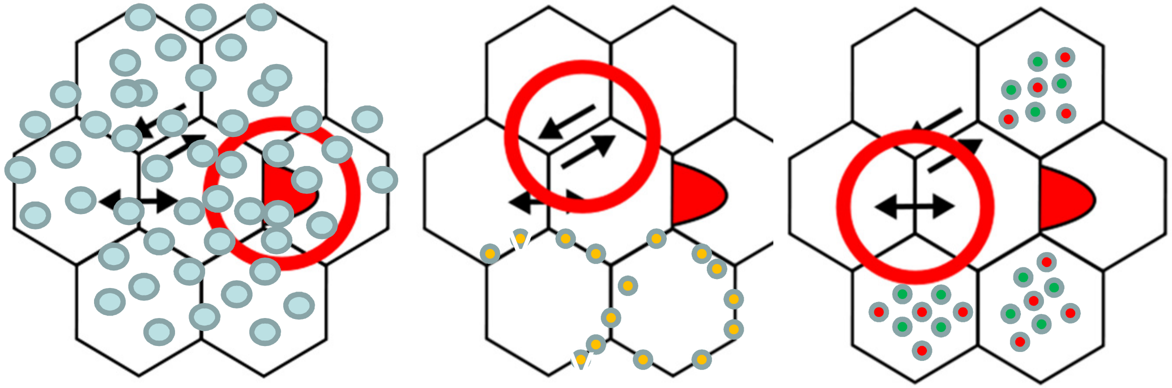
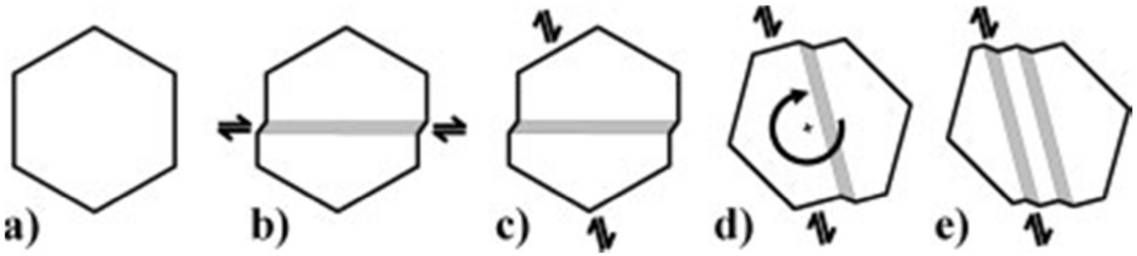
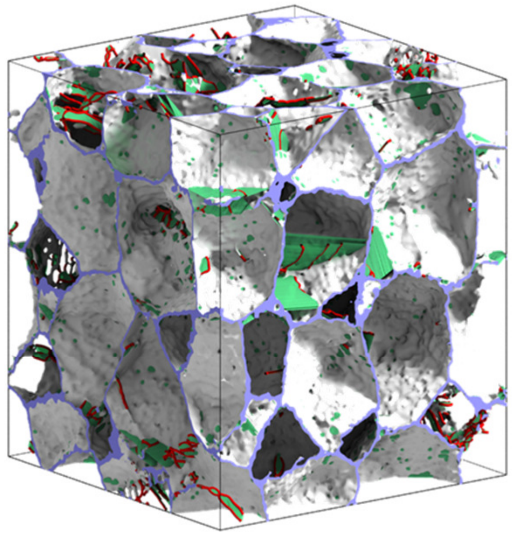
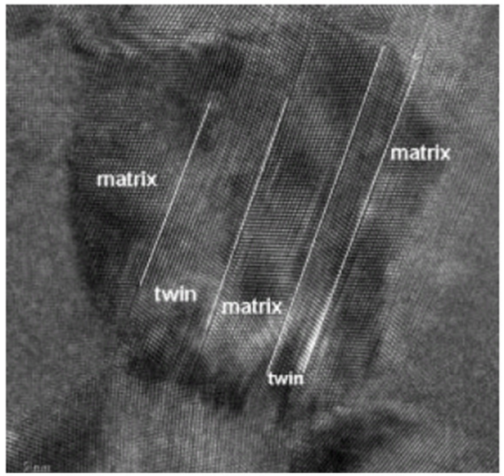


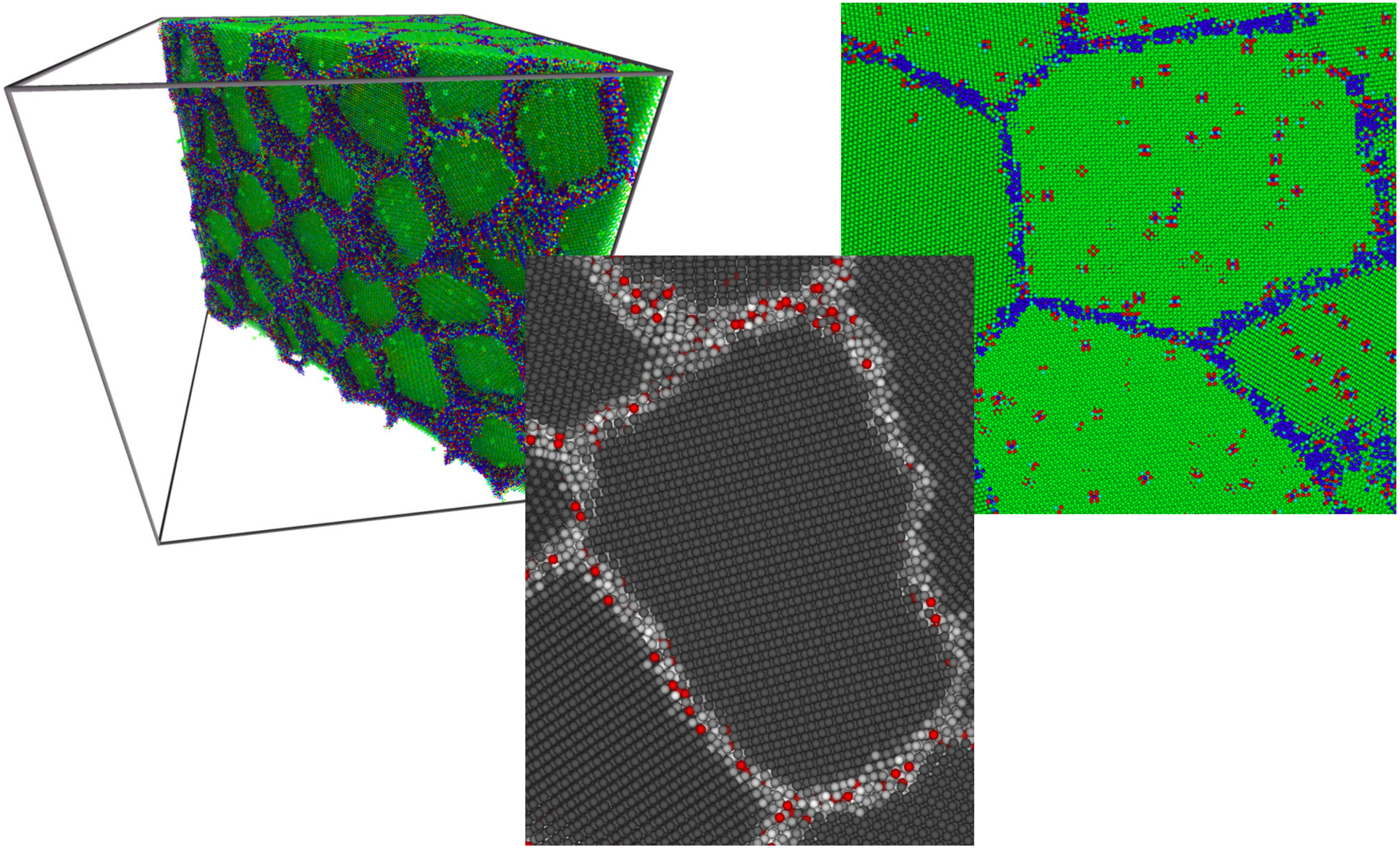






H. Rösner, J. Markmann, J. Weissmüller, *Philos. Mag. Lett.* **2004**, *84*, 321.

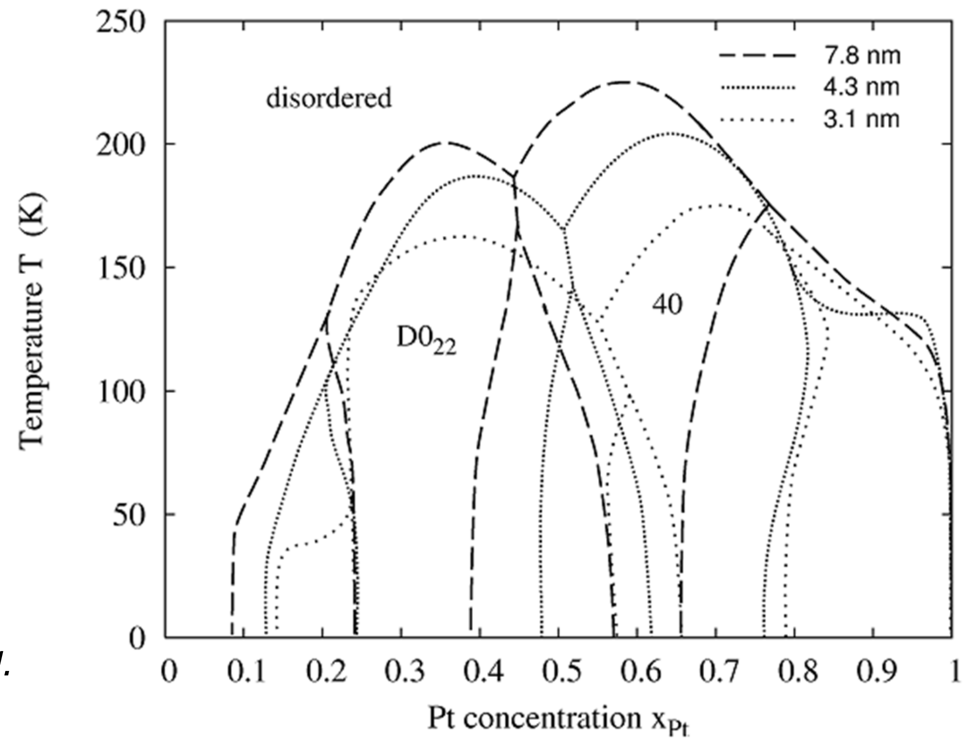
Distribution of solutes



MC-Algorithms

Canonical

$$\mathcal{A}_{\mathrm{C}} = \min\left\{1, \exp\left[-\beta \Delta U\right]\right\}$$

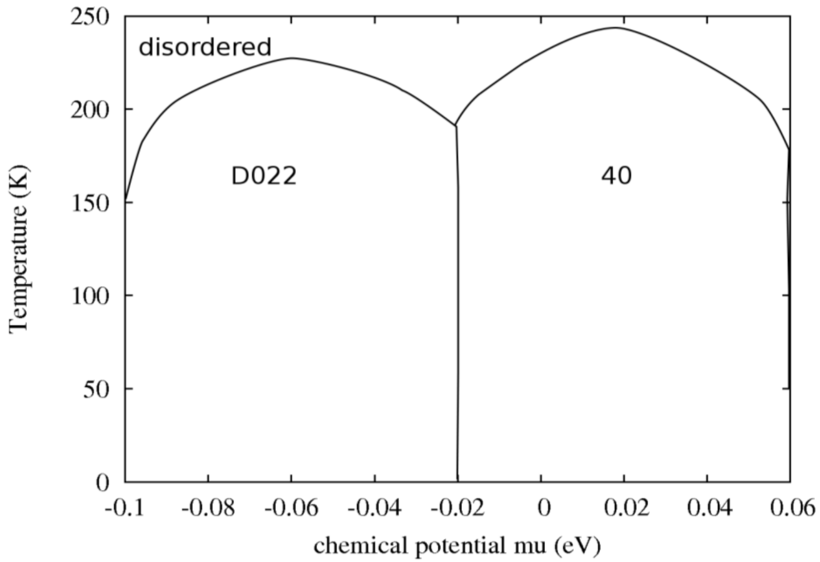


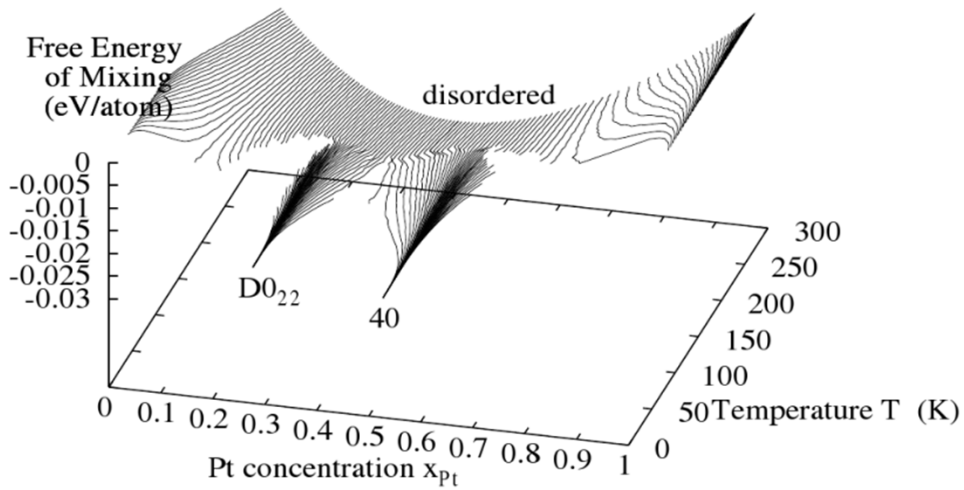
Pohl, Albe,
Beilstein J. Nanotechnol.
2012, *3,* 1–11

MC-Algorithms

Semi-Grandcanonical

$$\mathcal{A}_{\mathrm{S}} = \min\left\{1, \exp\left[-\beta(\Delta U + \Delta\mu N \Delta c)\right]\right\}$$

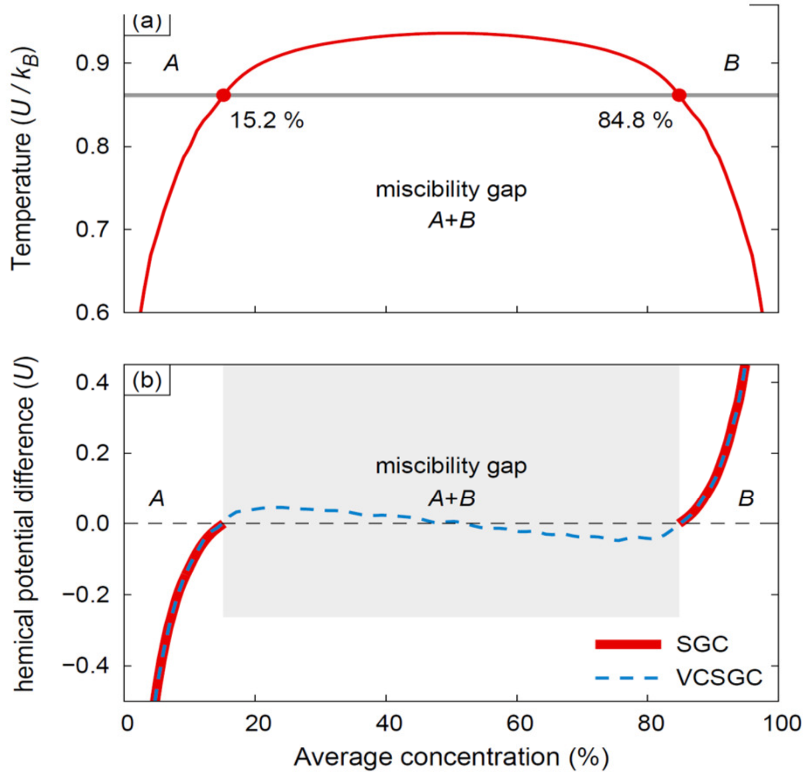




Variance constrained semi-grandcanonical scheme

$$\mathcal{A}_{\mathrm{V}} = \min\left\{1, \exp\left[-\beta\left(\Delta U + N\Delta c(\phi + 2\kappa N\tilde{c})\right)\right]\right\}$$

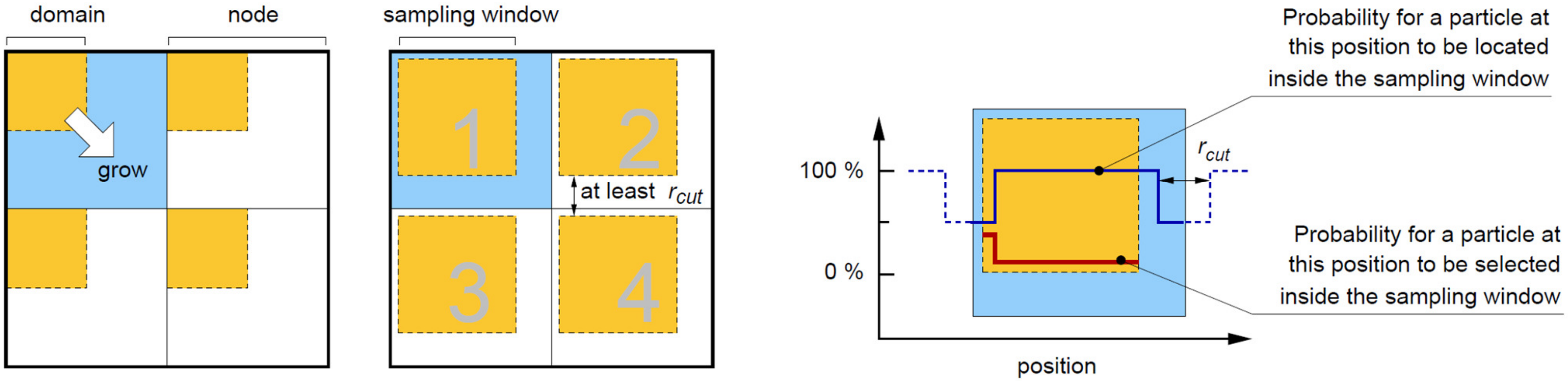
- The VCSGC-MC method imposes a constraint on the variance of the concentration, and allows for equilibration at arbitrary global concentrations.

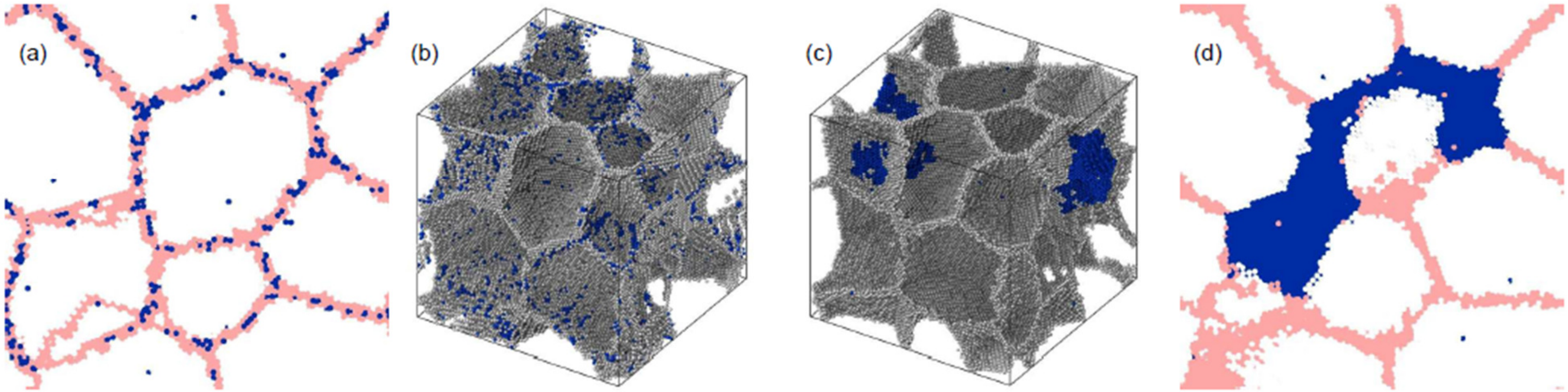


A scalable parallel Monte Carlo algorithm for atomistic simulations of precipitation in alloys

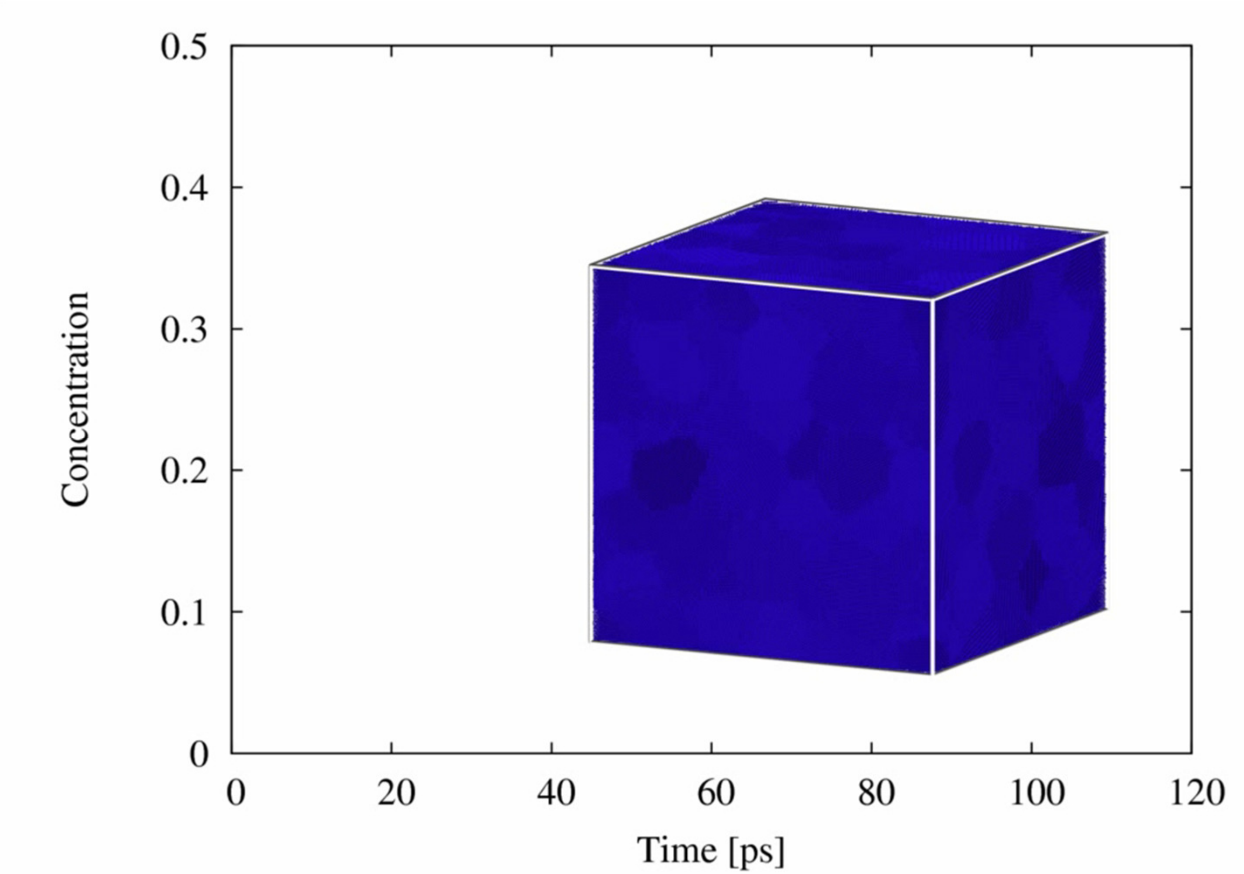
Babak Sadigh,[1,*] Paul Erhart,[1,†] Alexander Stukowski,[1] Alfredo Caro,[1,2] Enrique Martinez,[1,2] and Luis Zepeda-Ruiz[1]

Variance constrained semi-grandcanonical scheme: *Parallelization*





Annealing + Alloying: PdAu



Grain

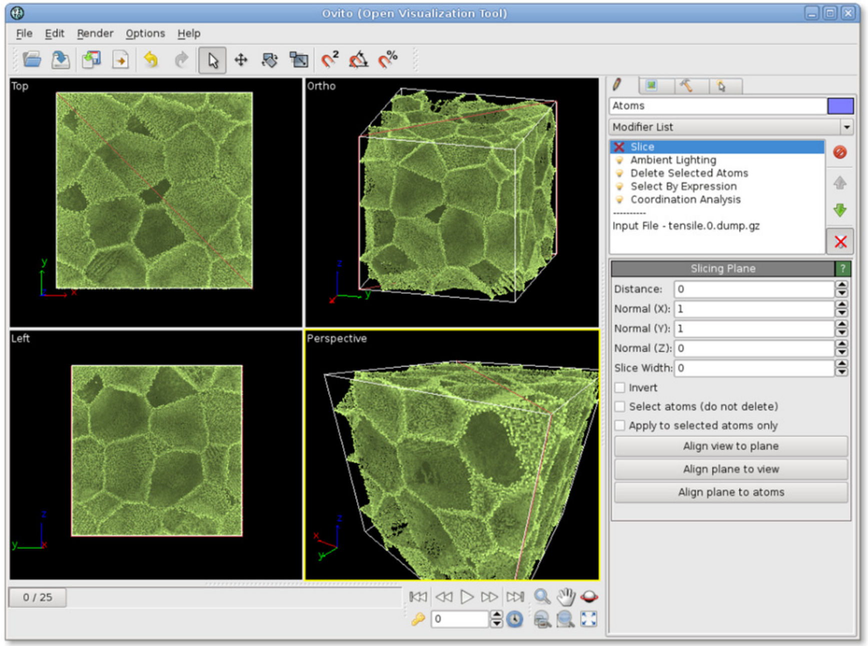
total

GB

OVITO
(Open Visualization Tool)

Visualization and analysis software for atomistic simulation data:

- Platform-independent
- Easy-to-use graphical user interface
- Extendable (plug-in architecture)
- Supports scripting / batch-processing
- >110.000 lines of code (C++)
- Freely available at http://ovito.org/



A. Stukowski,
Modelling Simul. Mater. Sci. Eng. 18, 015012 (2010)

Dislocation Analysis: The challenge

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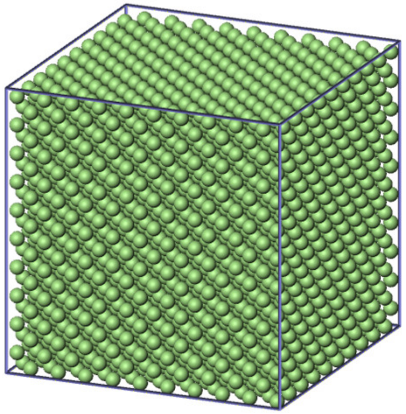
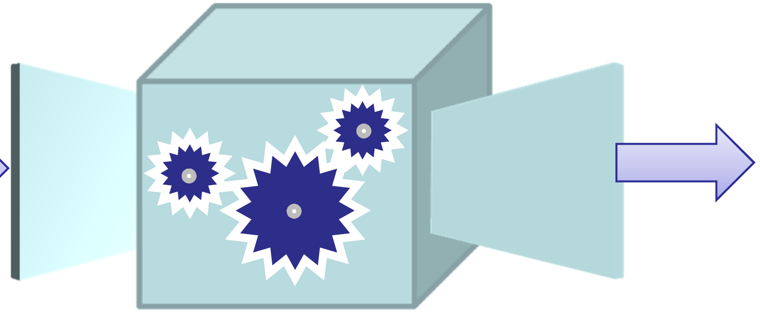
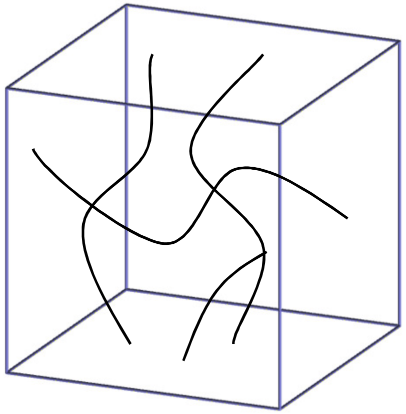


Input:
Atomic coordinates





Output:
Discrete dislocation lines
+ Burgers vectors

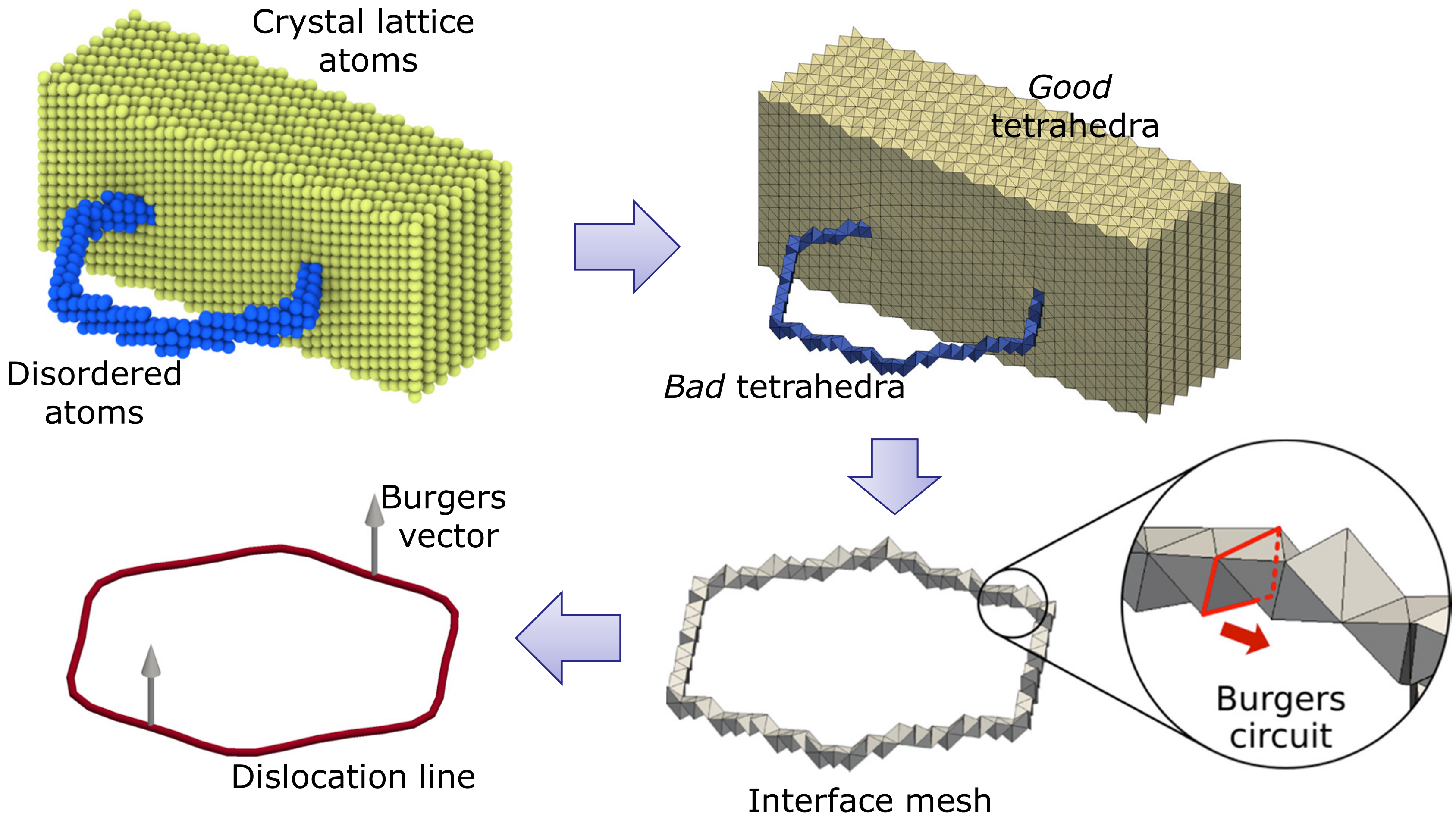
Handle arbitrary Burgers vectors
+ polycrystals

Extract complete networks of dislocations

Partial dislocations
+ twinning dislocations

Do it on the fly
+ parallel

Dislocation Extraction Algorithm (DXA)

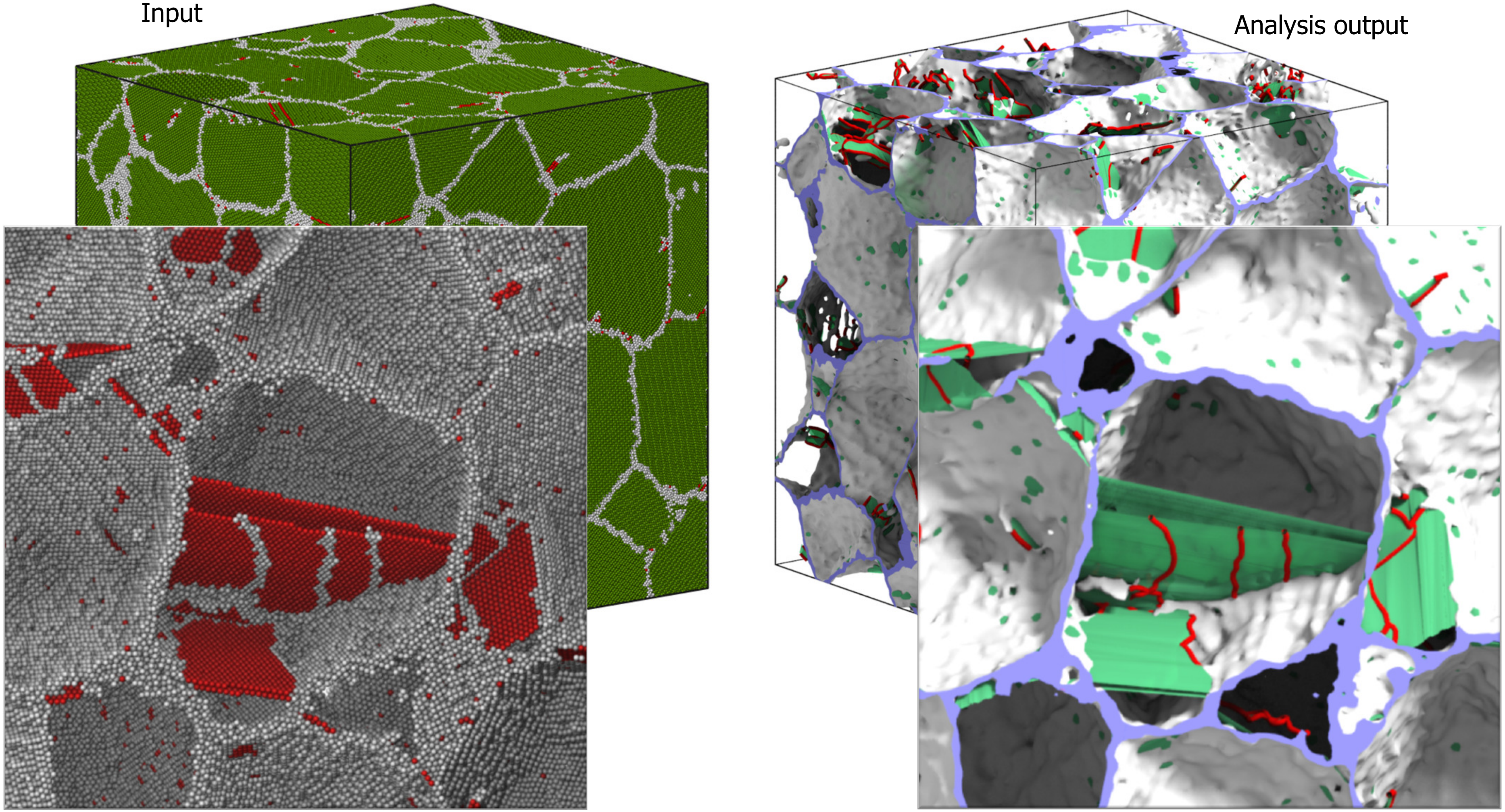


Stukowski & Albe,
Modelling Simul. Mater. Sci. Eng. 18 (2010), 085001

Stukowski, Bulatov, Arsenlis,
Modelling Simul. Mater. Sci. Eng. 20 (2012), 085007

Example: Nanocrystalline microstructures under deformation

Nanocrystalline Pd



Automated dislocation detection

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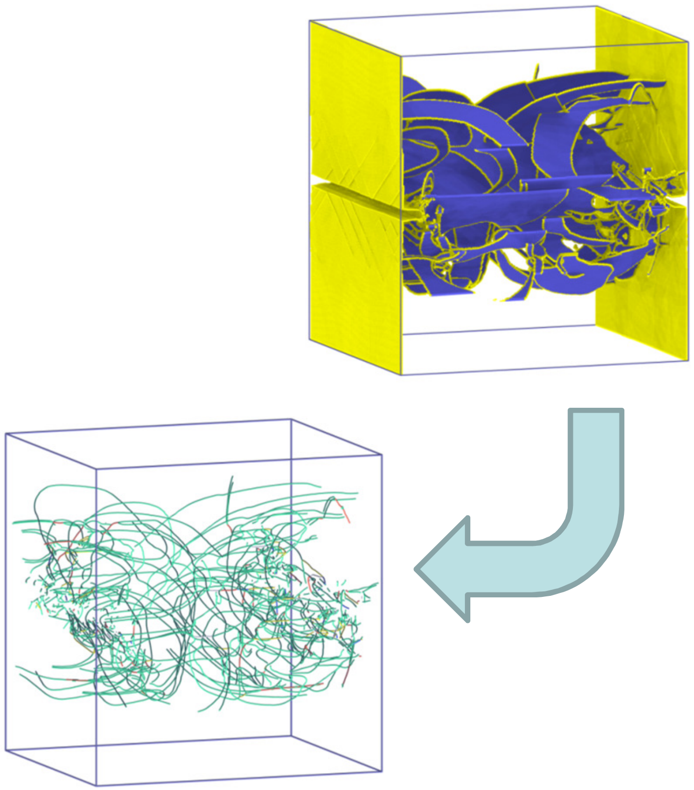
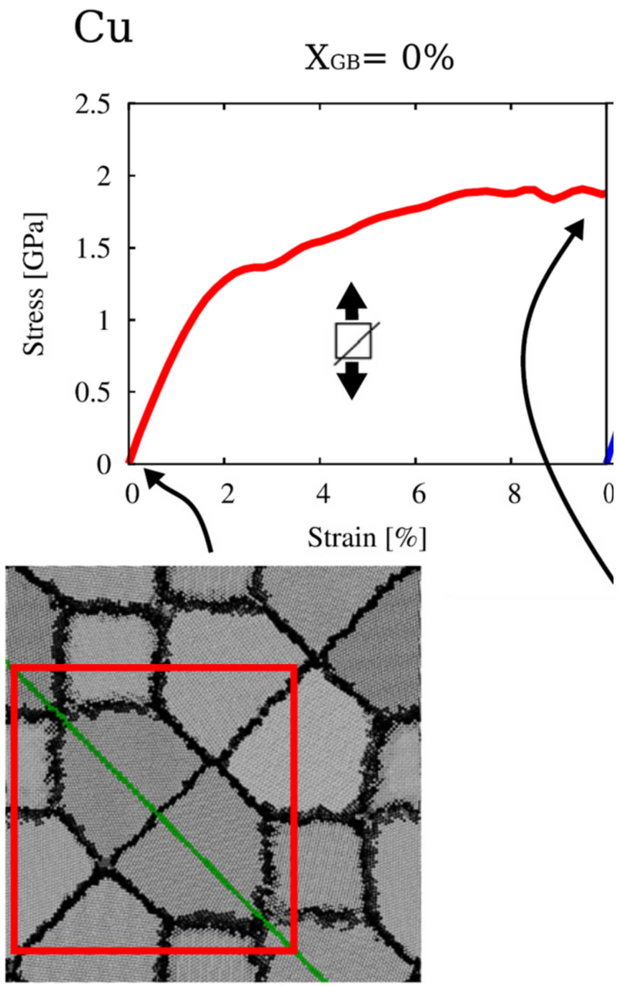
What can we do with it?

- Measure..
  - Dislocation density
  - Dislocation characters
  - Activation rate of slip systems
  - Types of dislocation junctions
  - ...
- Reduce output data size (by ~99.9 %)
- Link MD to other models...
  - Discrete dislocation dynamics (DD) models
  - Continuum plasticity models
    (via dislocation density tensor)



Coupled Motion vs. Sliding:
nc Cu-Nb (10nm)



Coupled Motion vs. Sliding:
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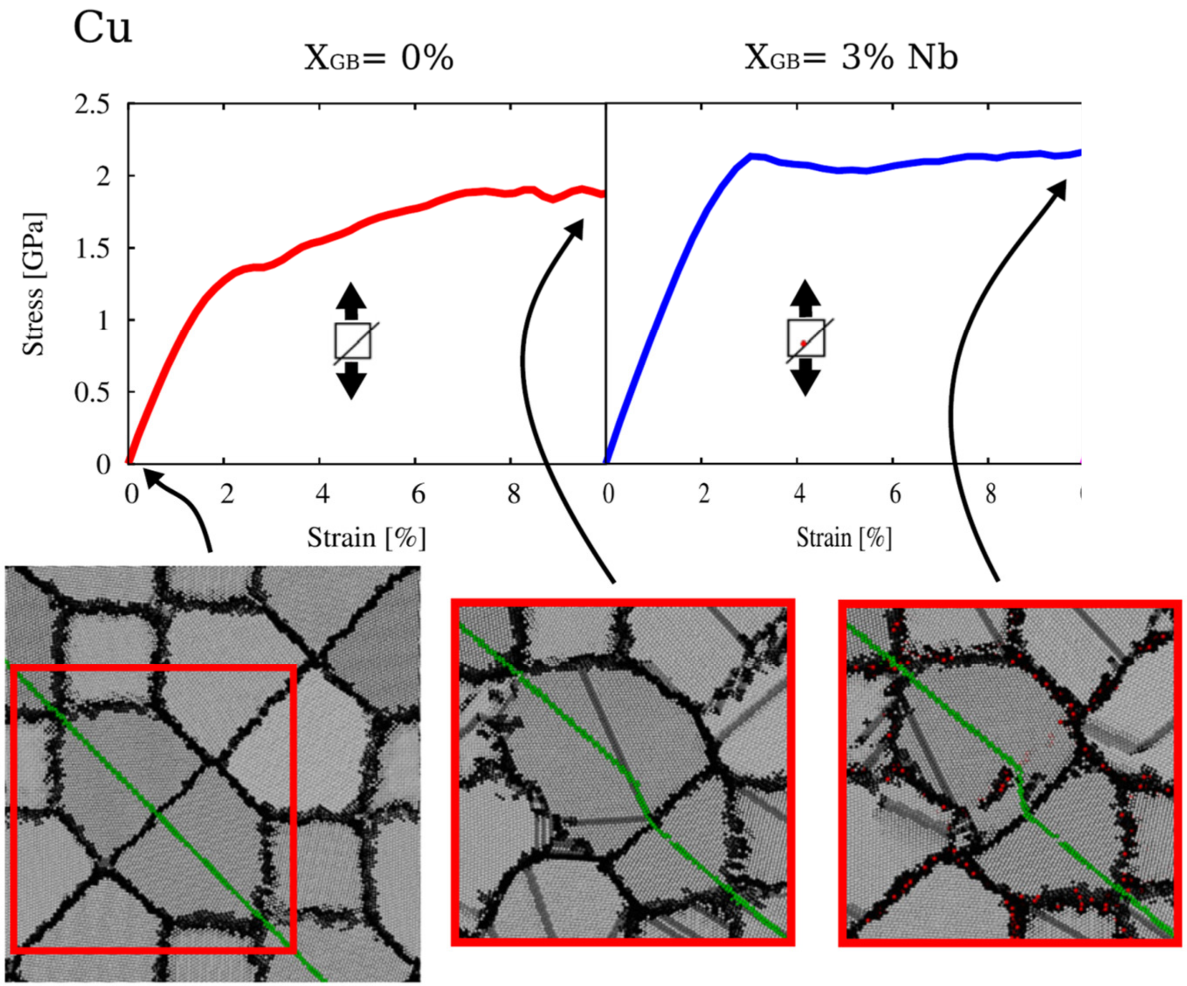
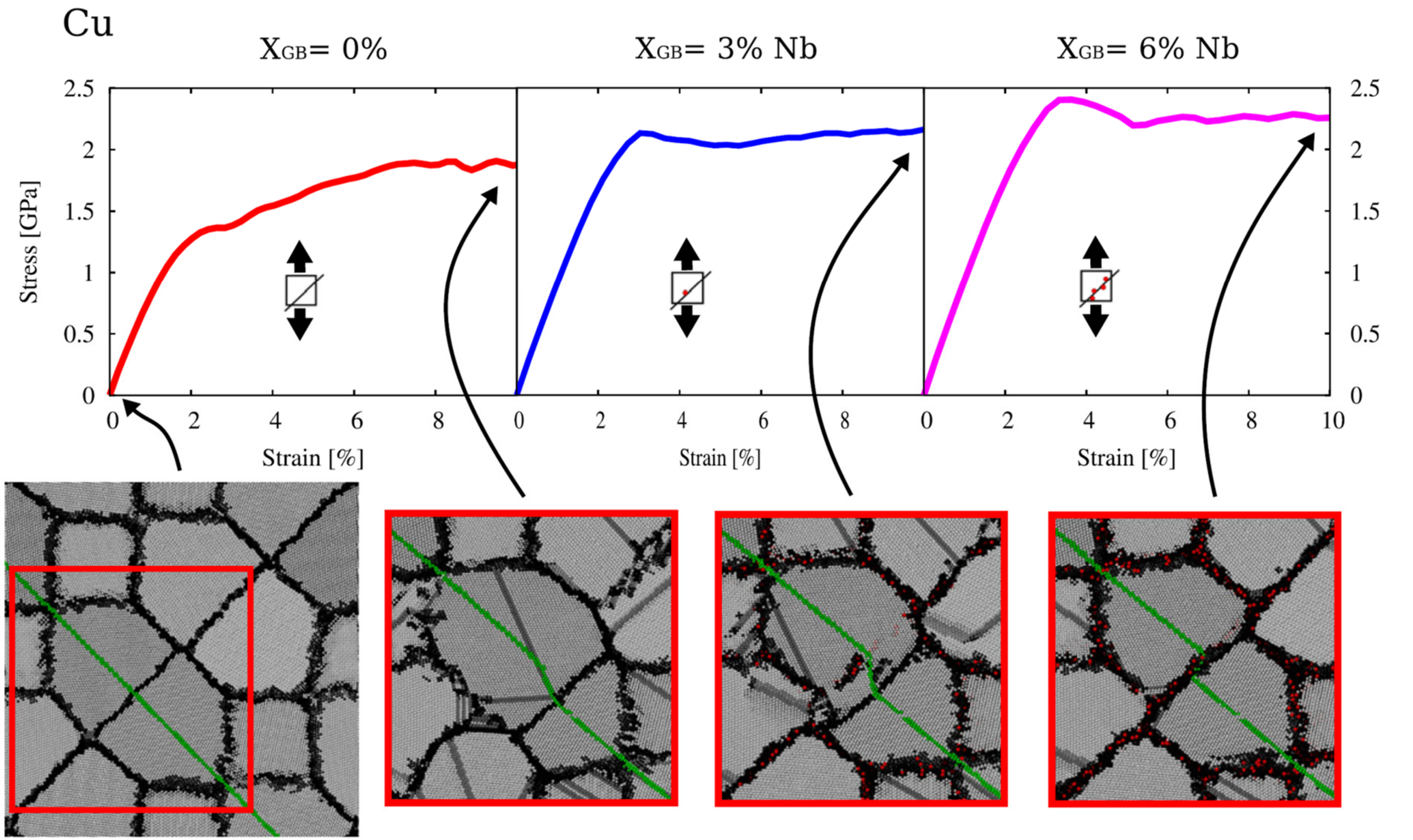


Coupled Motion vs. Sliding: nc Cu-Nb (10nm) randomly alloyed

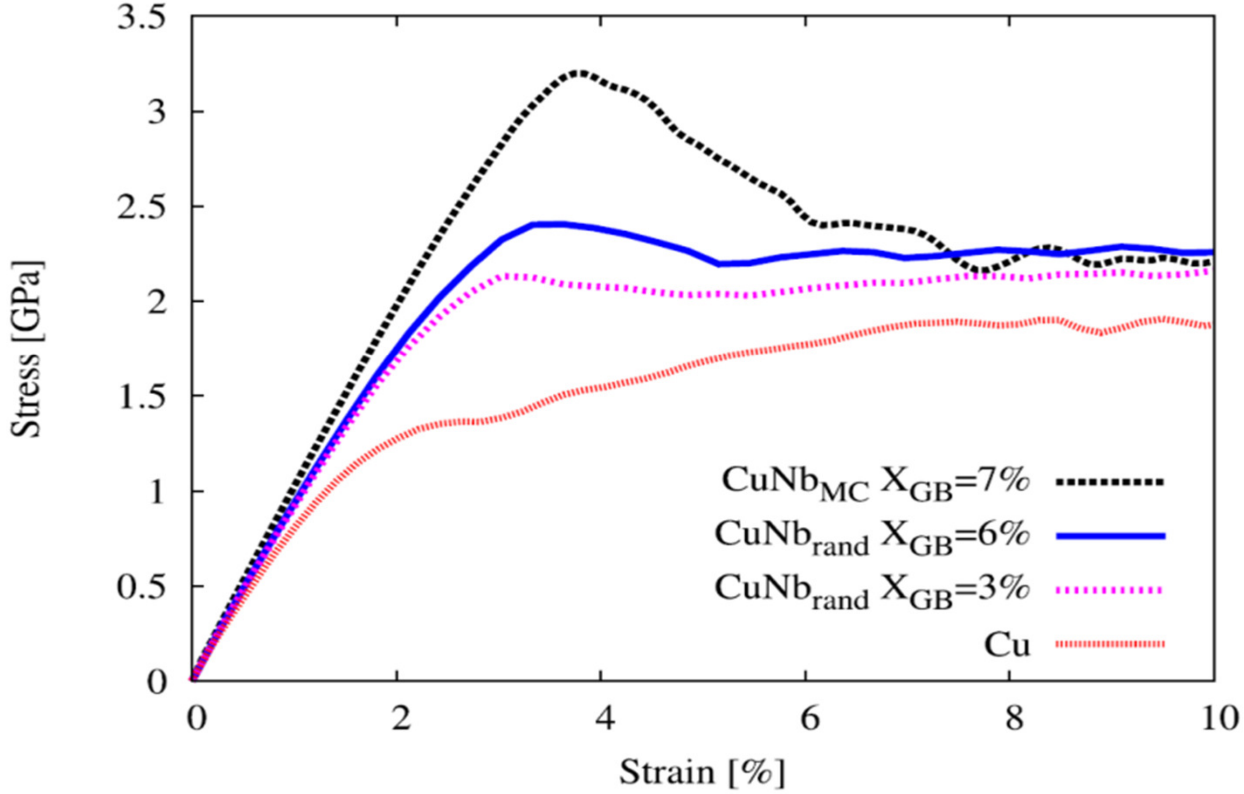


Schäfer, Albe, Sripta Materialia, 66 (5) pp. 315-317, 2011

Coupled Motion vs. Sliding: State GB Relaxation State

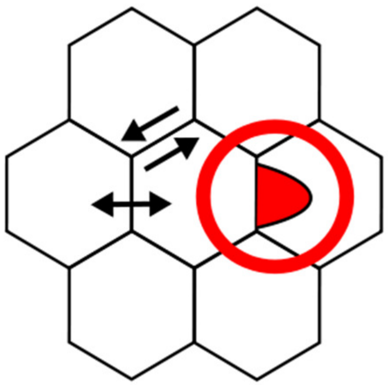
Randomly alloyed GBs

Equilibrated GBs



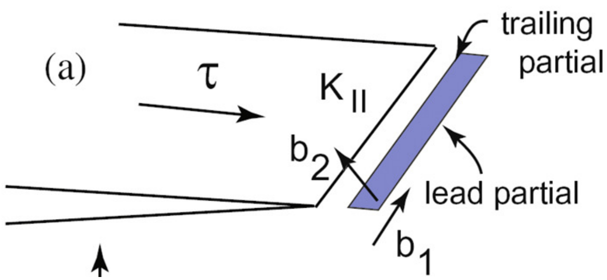
Schäfer, Albe, Acta Mat, 60, 6076 (2012)

Dislocation nucleation

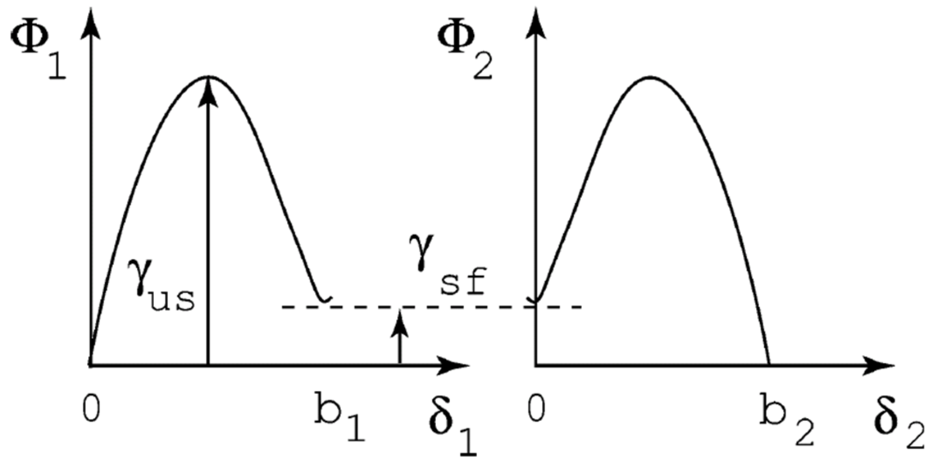


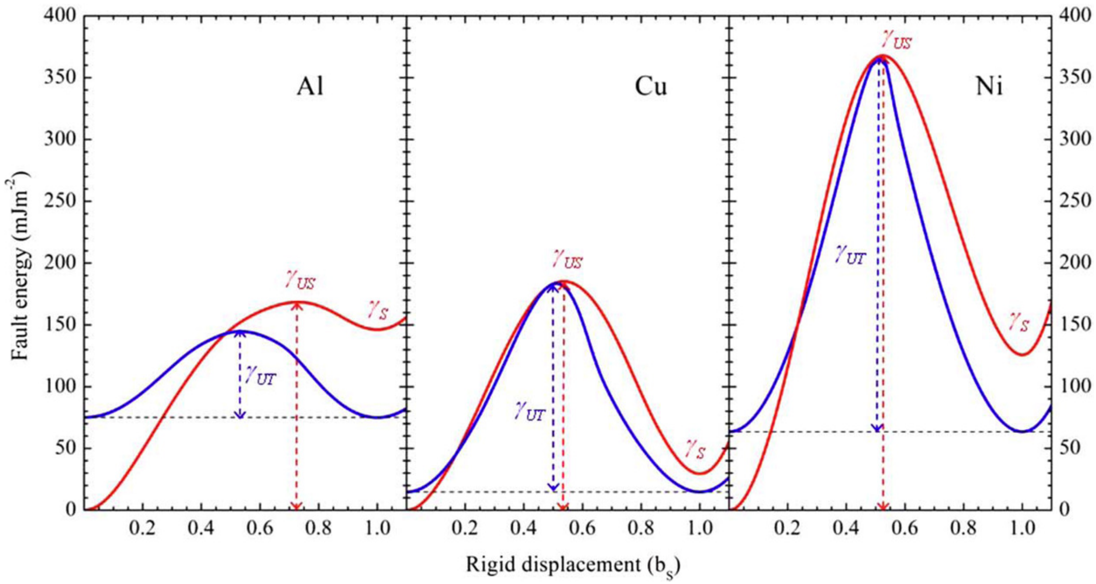
$R = (\gamma_{usf})/Gb$

Asaro, Suresh, Acta Mater., 53 (2005)



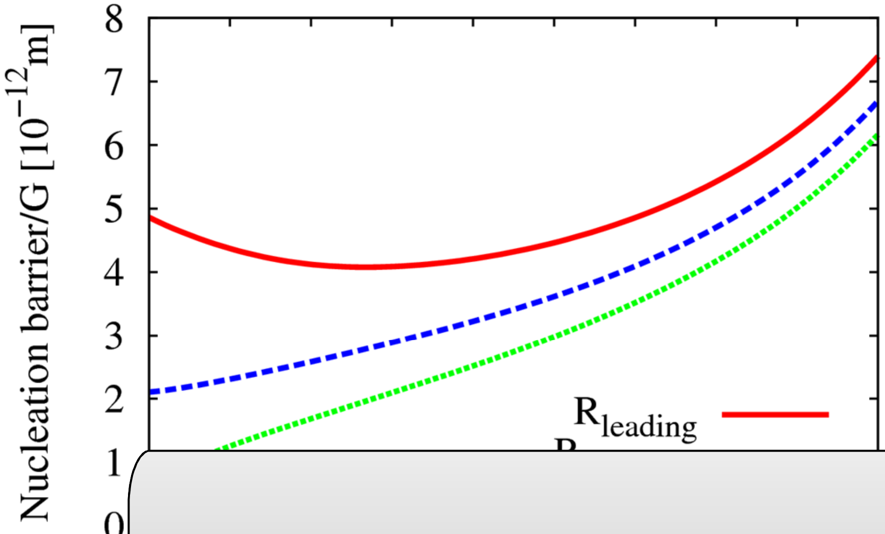
Rice, J. Mech. Phys. Solid., 40 (1992)



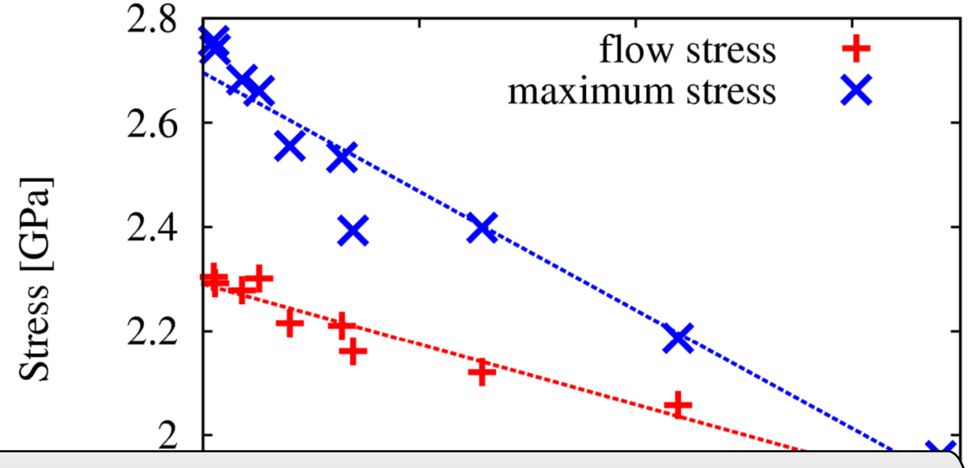


PdAu: alloying effects

$R = (\gamma_{usf})/Gb$



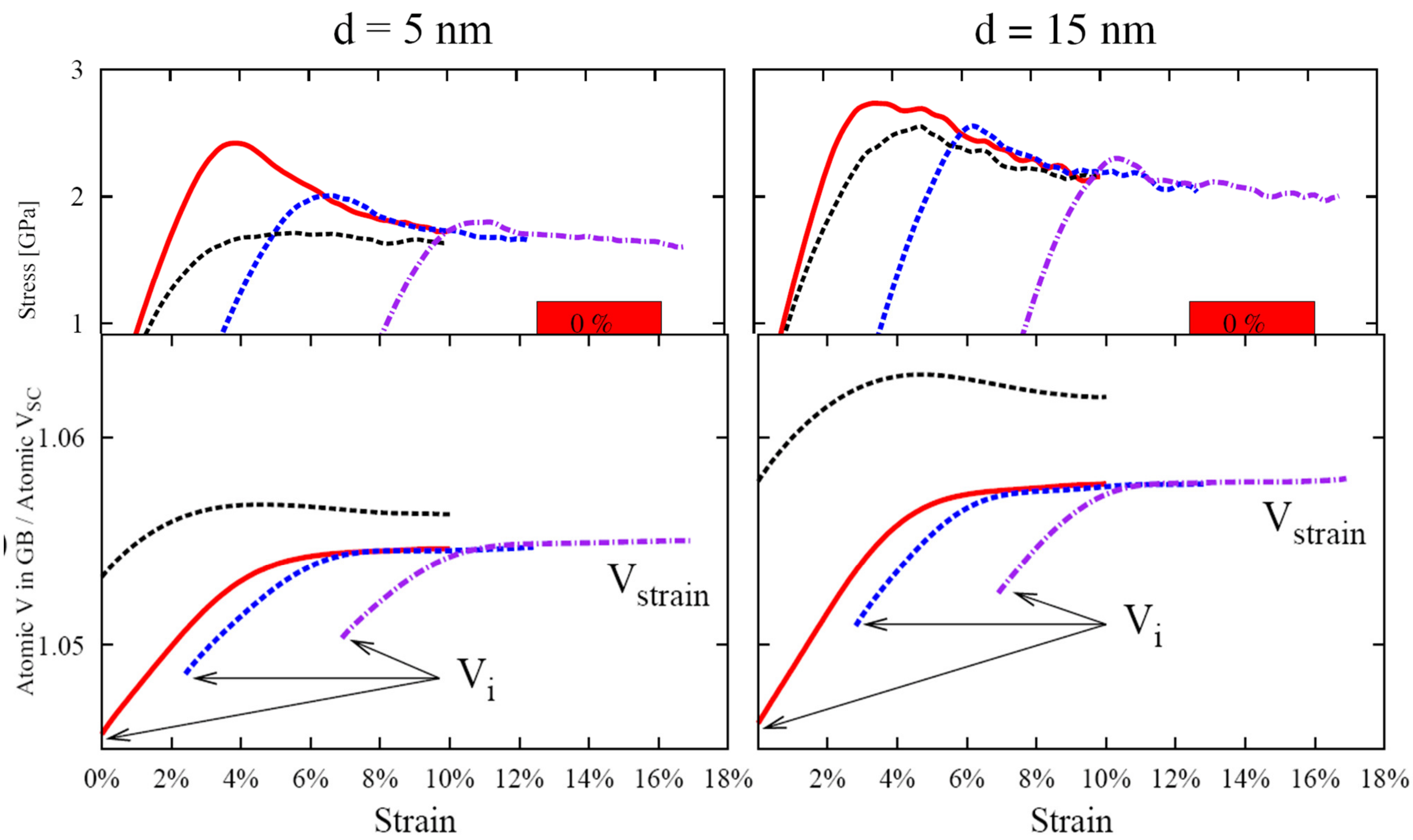
15 nm



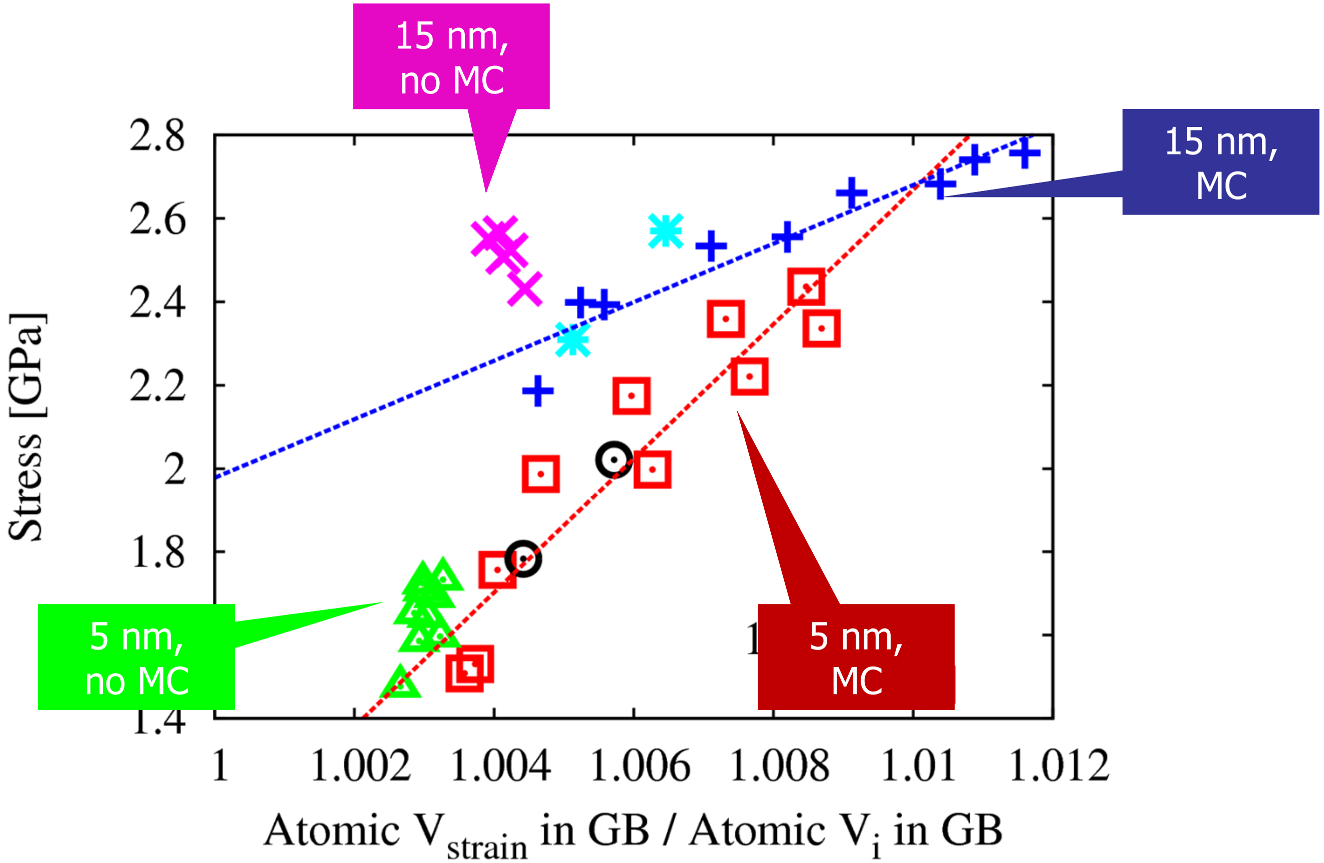
Dislocation nucleation barrier cannot explain increased maximum stress. What are the atomistic reasons?

Schäfer et al., Acta Materialia, 59, (2011)

Role of GB equilibration and reloading

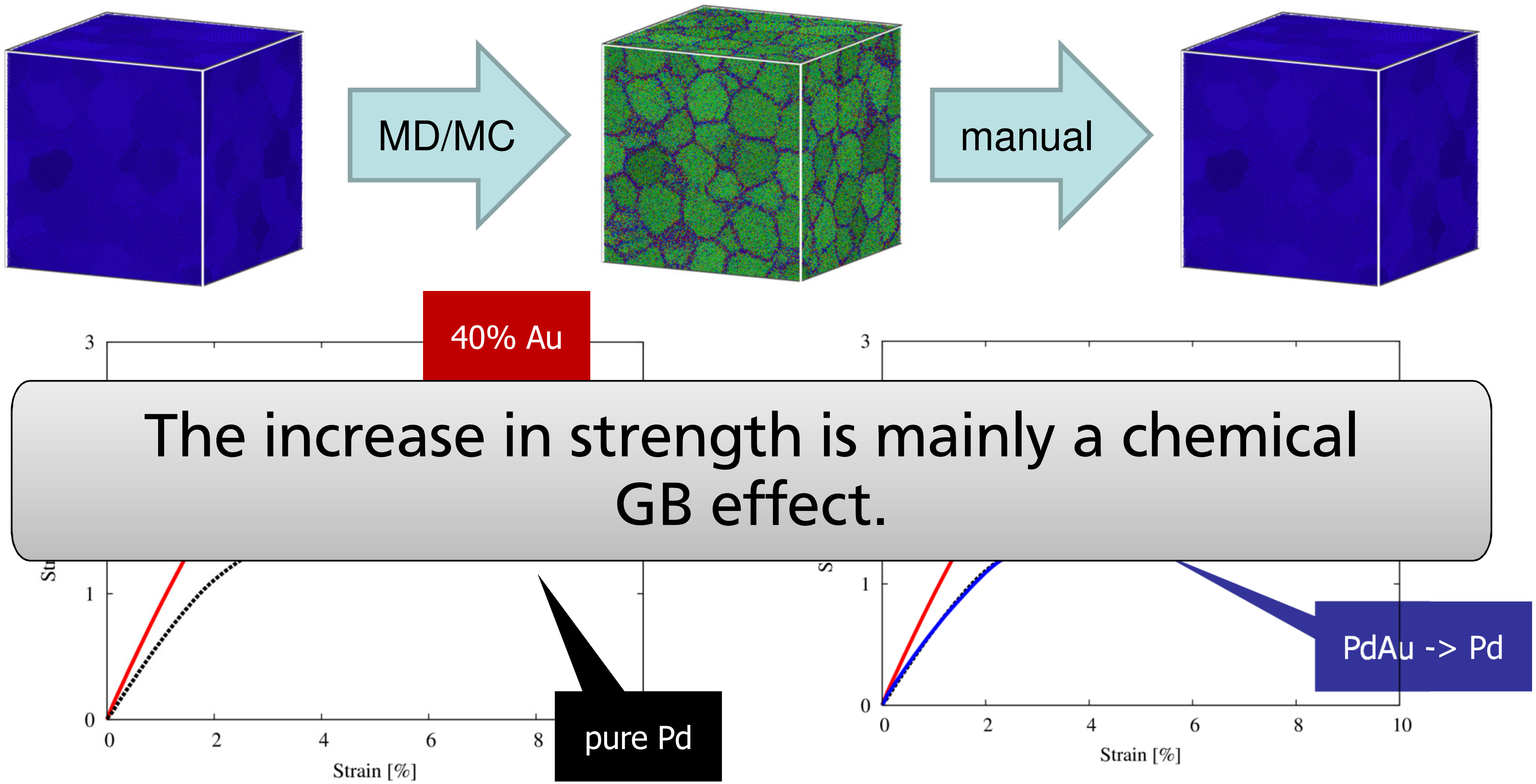


PdAu: equilibration effects



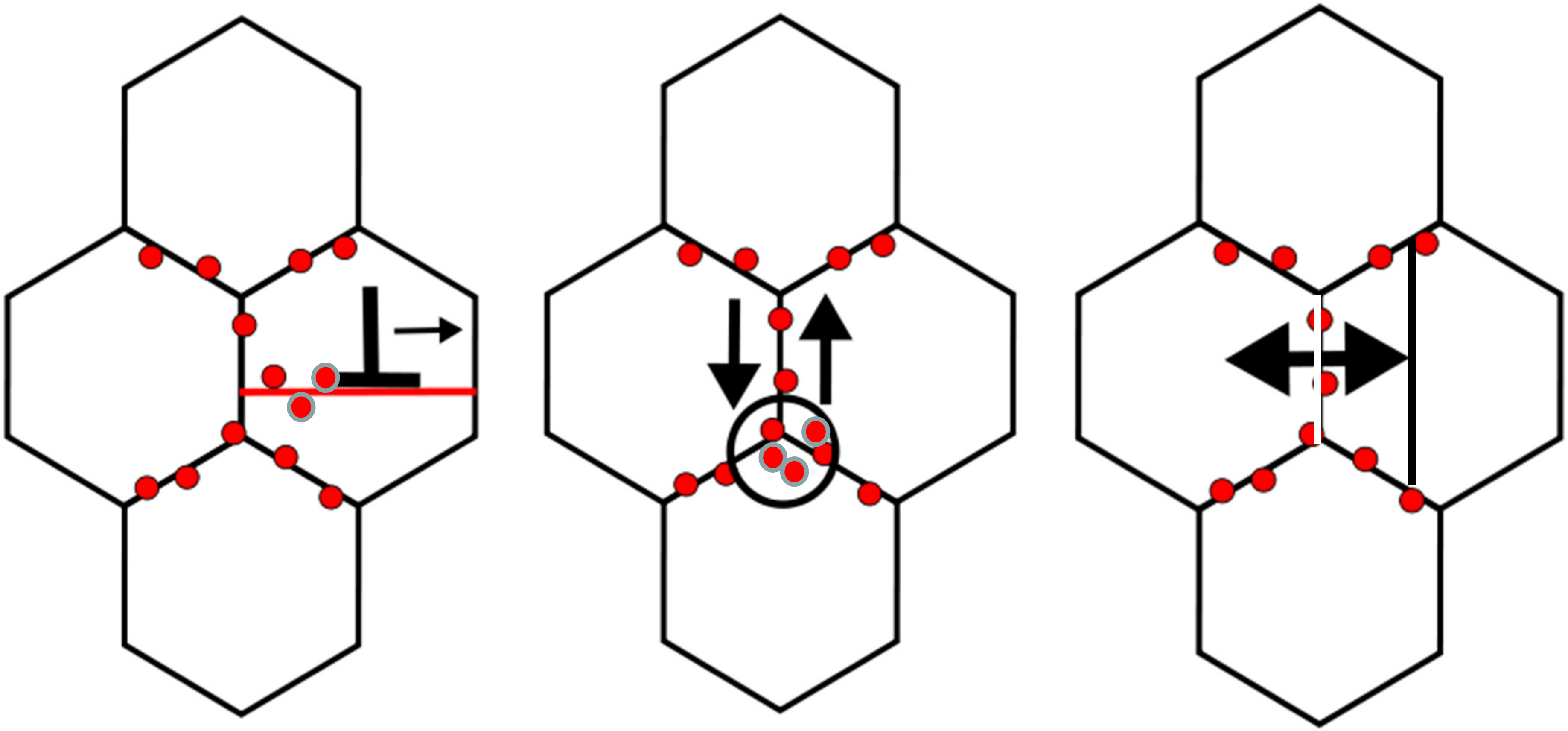
Schäfer et al., Acta Materialia, 59, (2011)

PdAu: Equilibration effects ?

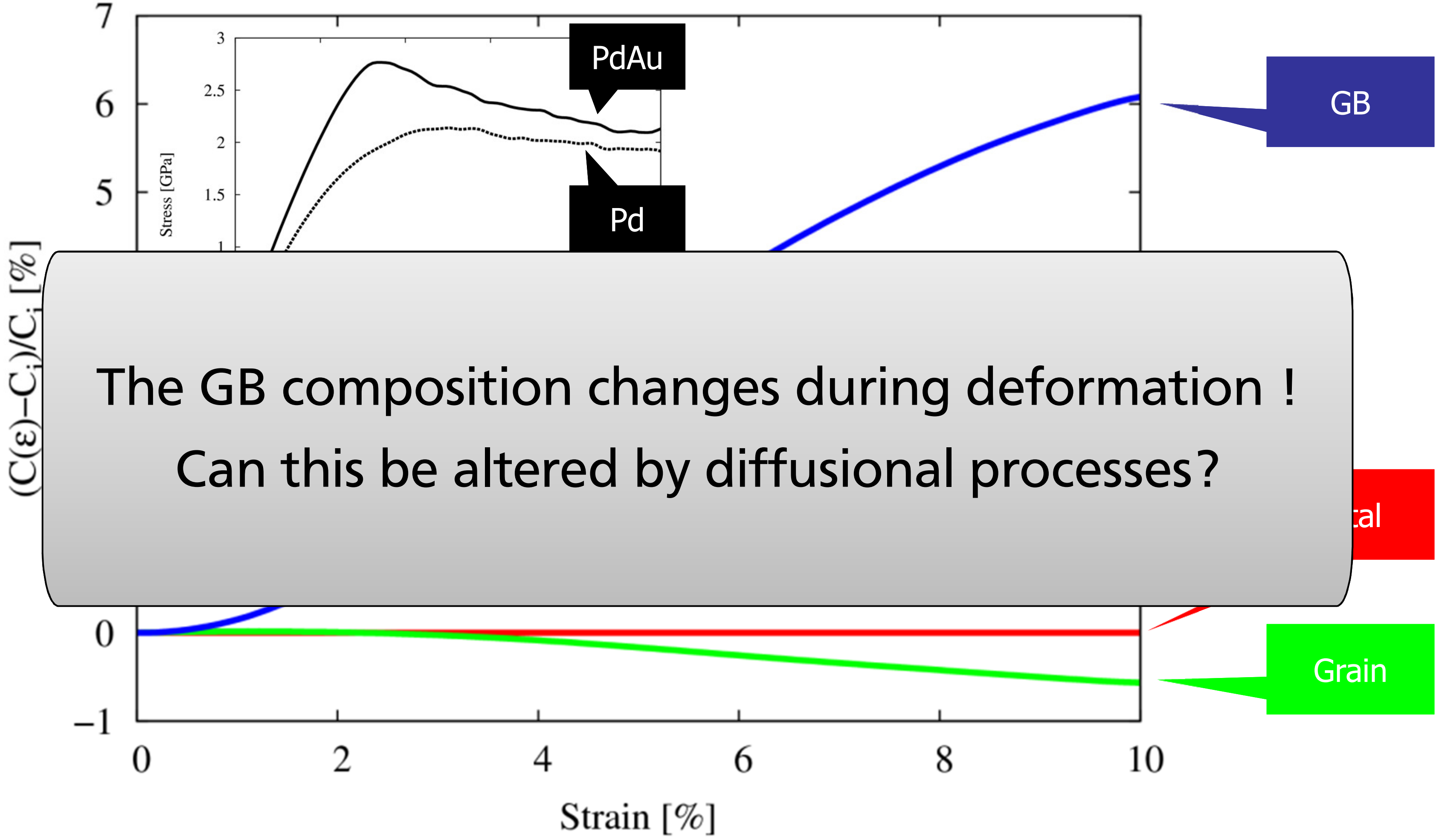


The increase in strength is mainly a chemical GB effect.

Redistribution of Solutes?



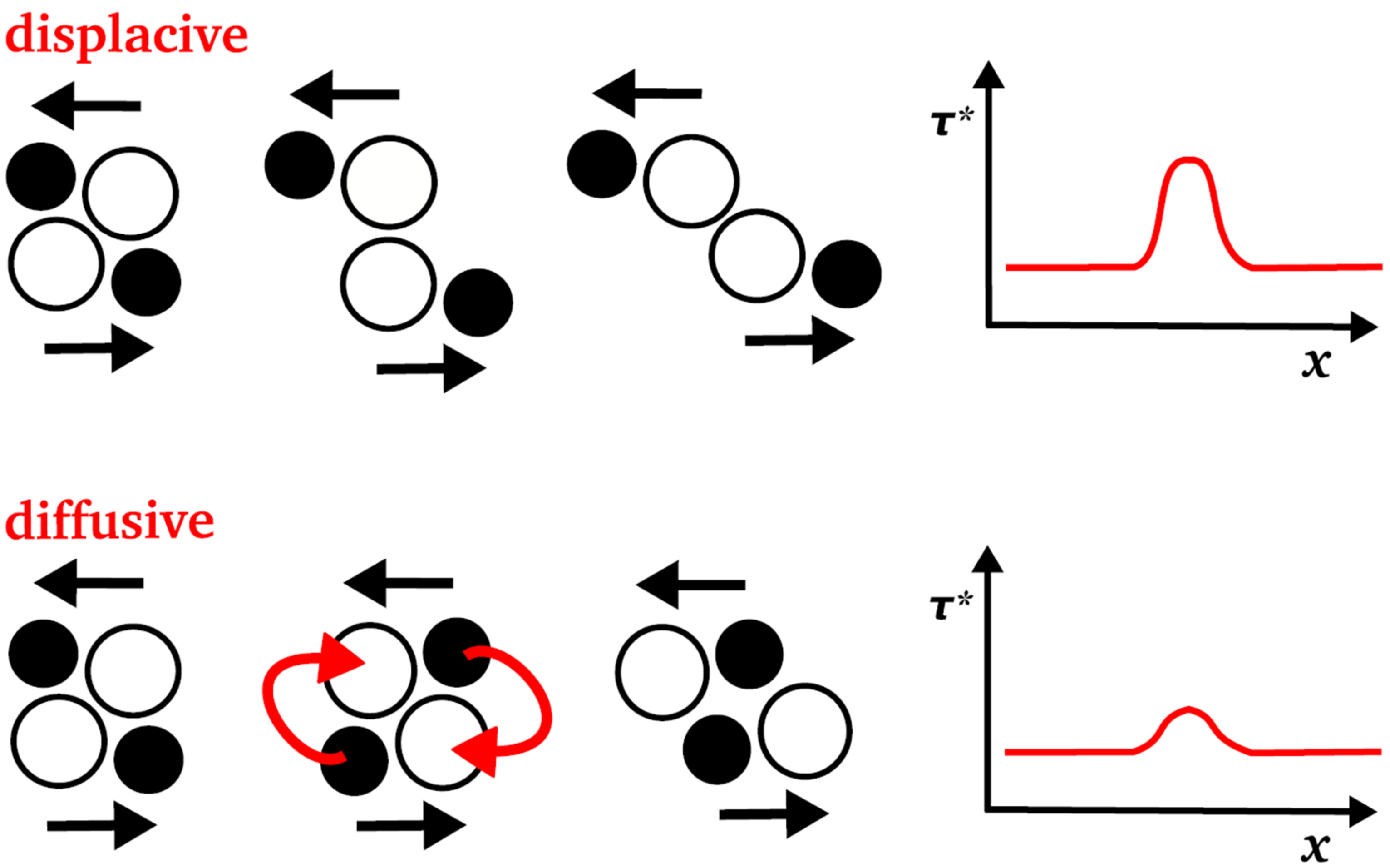
GB composition during straining



The GB composition changes during deformation !

Can this be altered by diffusional processes?

Studying Strain Rate Effects: Stortcutting Diffusion



Shortcutting Diffusion

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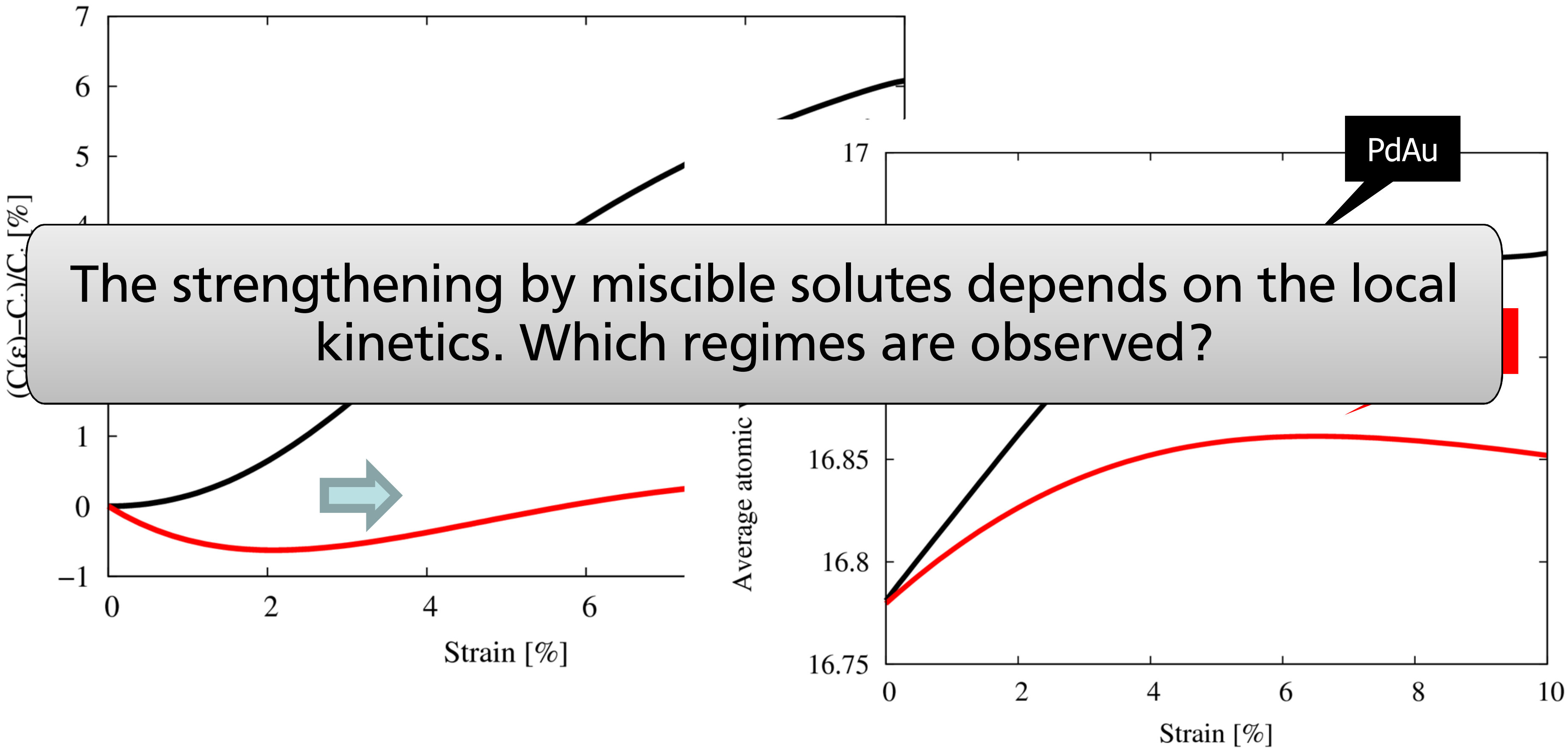

The strengthening by miscible solutes depends on the local kinetics. Which regimes are observed?

Overshoot and Reversible Strain (MD)

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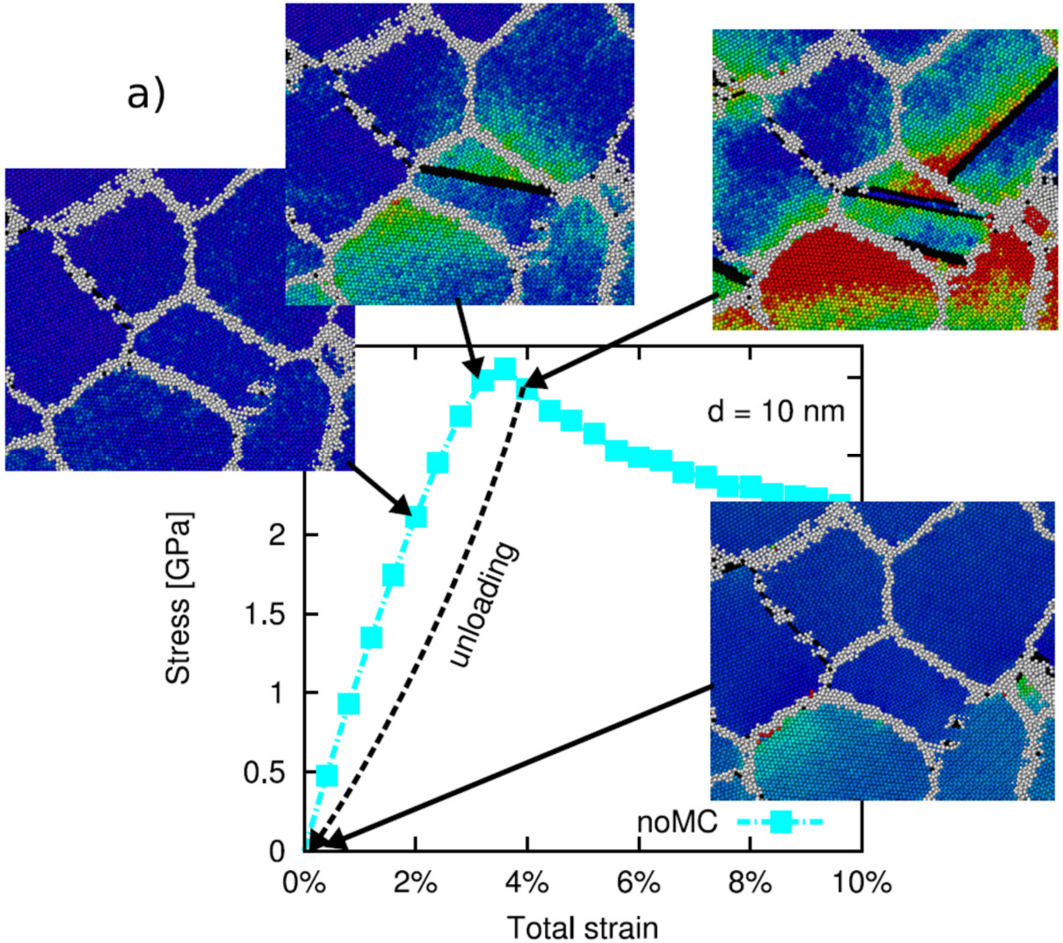
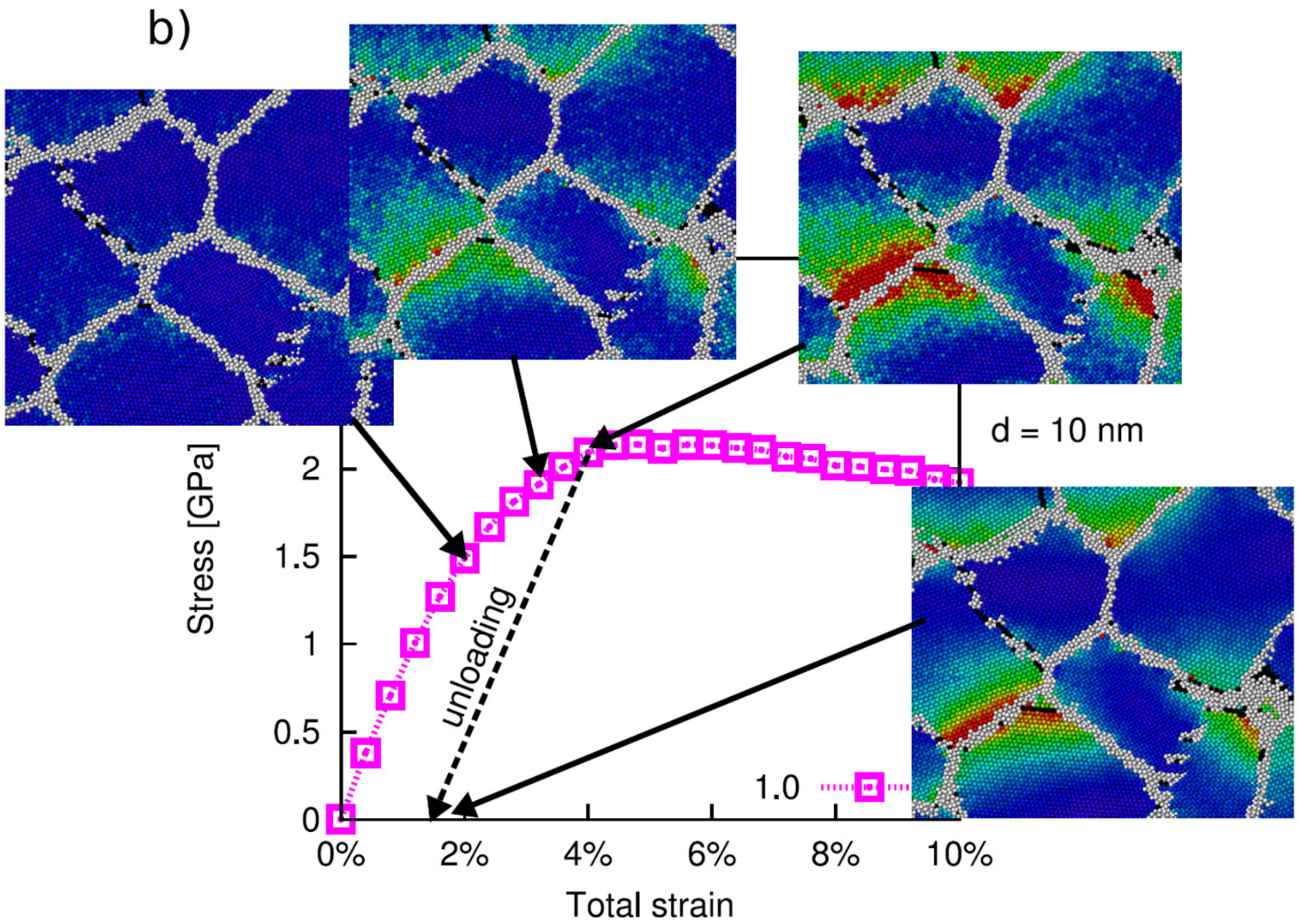
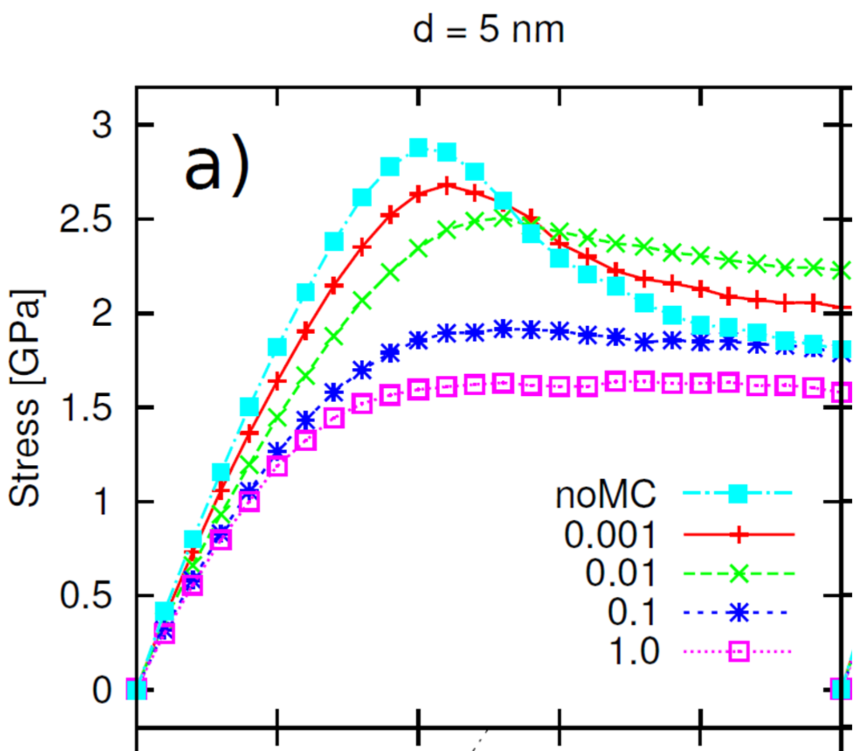
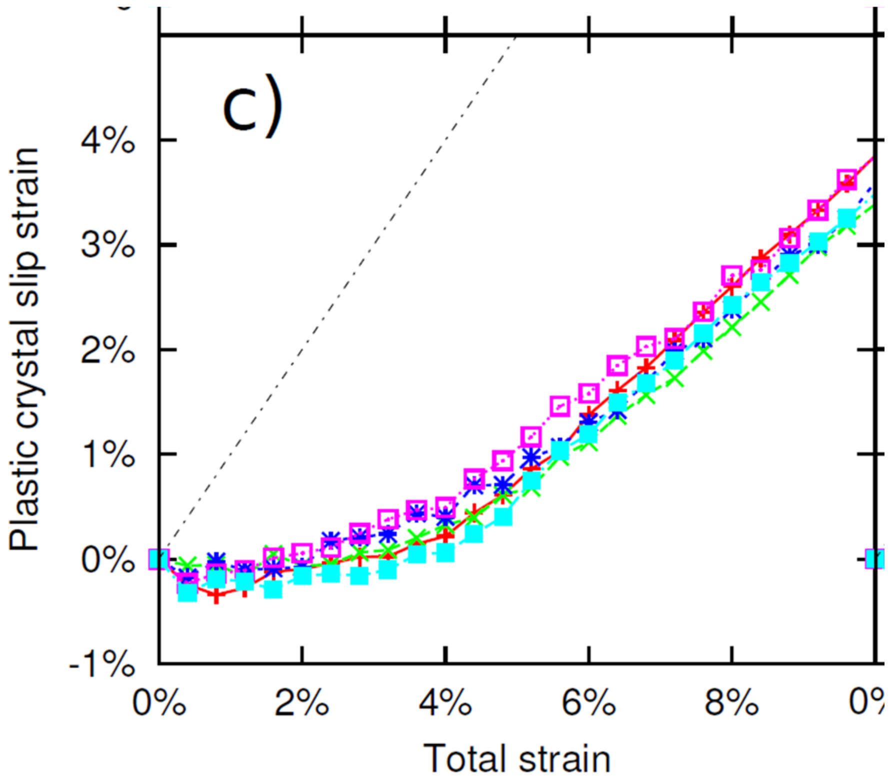


Overshoot and Reversible Strain (MD/MC)



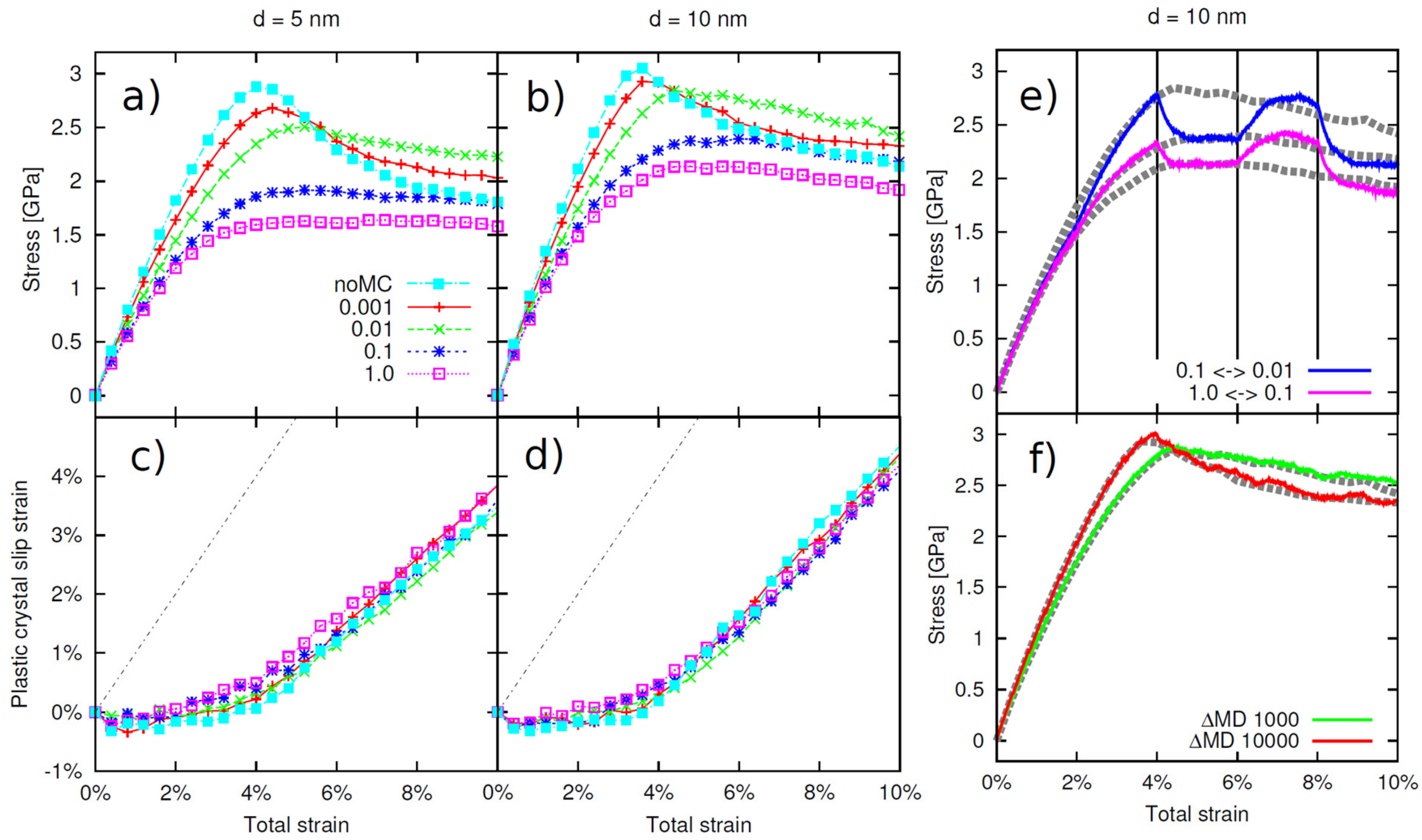
Mimicking „Strain-Rate“ Effects





Schäfer, Stukowski, Albe, J. Appl. Phys. *In print*

Mimicking „Strain-Rate“ Effects



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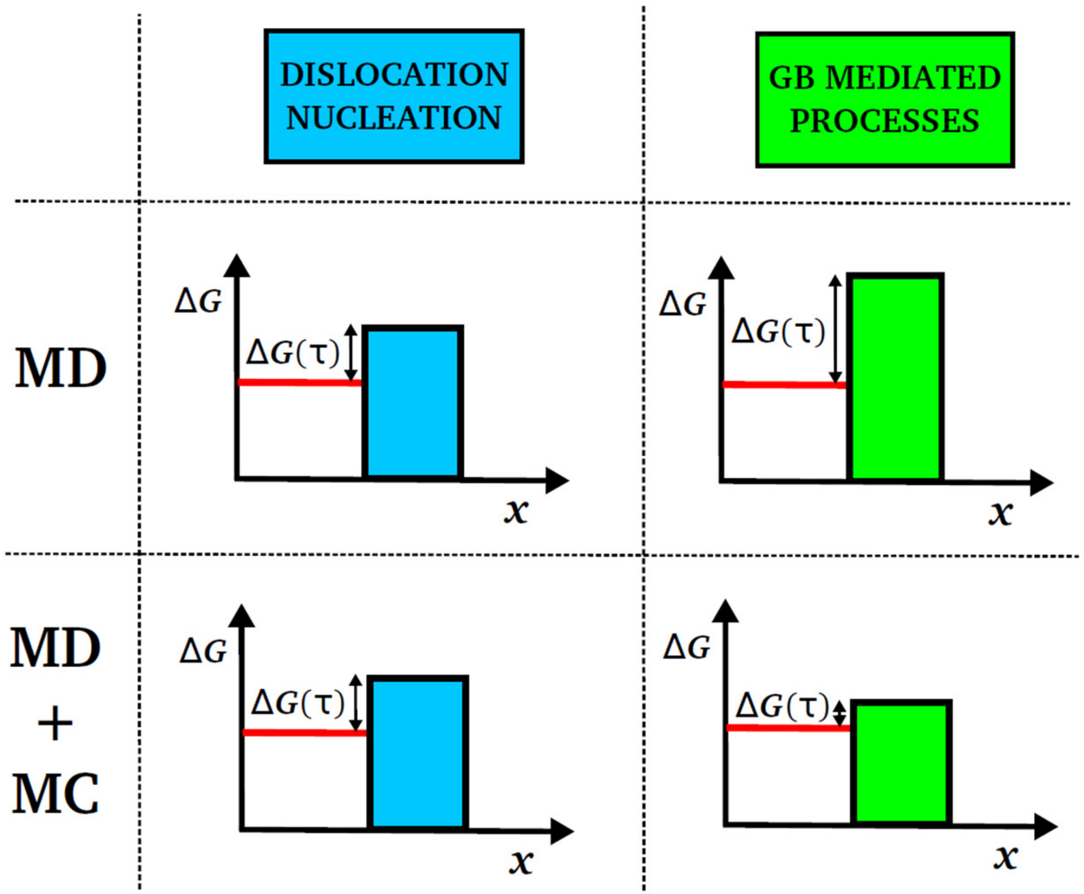
Shortcutting diffusion



Conclusions

- MD simulations are in principle a powerfull tool to investigate mechanical deformation mechanisms in detail, but are limited due to large strain rates and thus„diffusionless“ conditions

- Hybrid MD/MC simulations reveal that

  - the GB state not the grain interior governing the plastic response of nanocrystalline alloys

  - MD simulations overestimate the slip contributions of dislocations

- There is an urgent need to quantitative methods that allow accerated MD/KMC simulations