# Deformation behaviour of nanocrystalline alloys simulated by *Hybrid MD/MC simulations*

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# Outline

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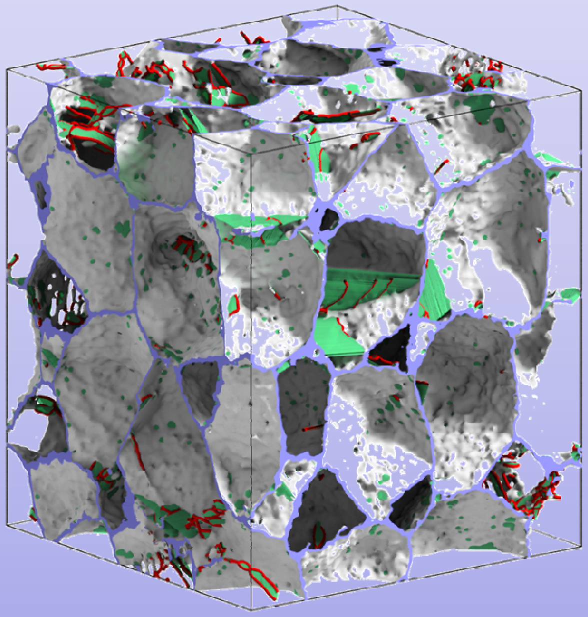
Motivation: Deformation of nanocrystalline metals

Nanocrystalline Pd-Au:

- *Hybride MD-MC Scheme*
- Method for dislocation detection: *DXA*
- Shortcutting diffusion
- Coupled motion



# Strengthening metals and alloys

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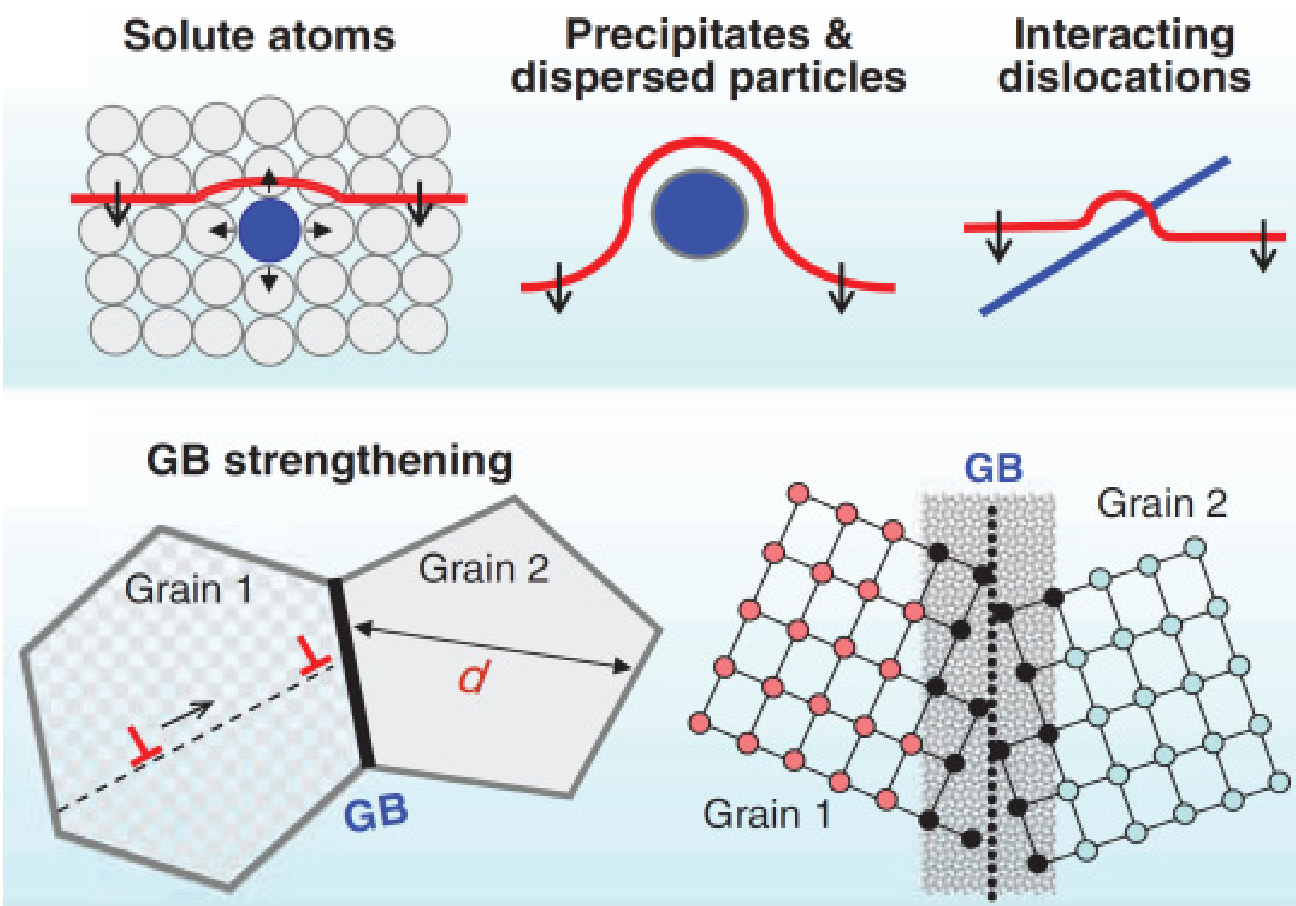


# Nanocrystalline metals

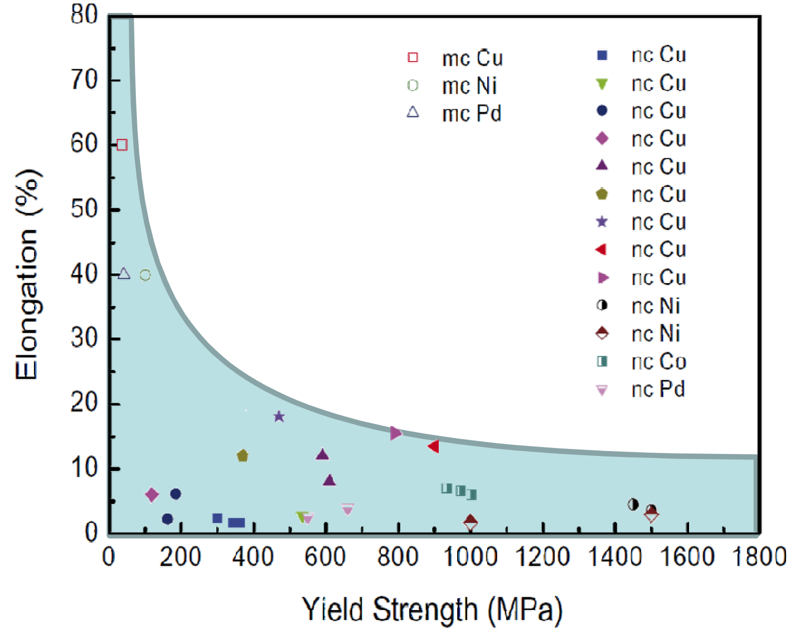
## Microstructure

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

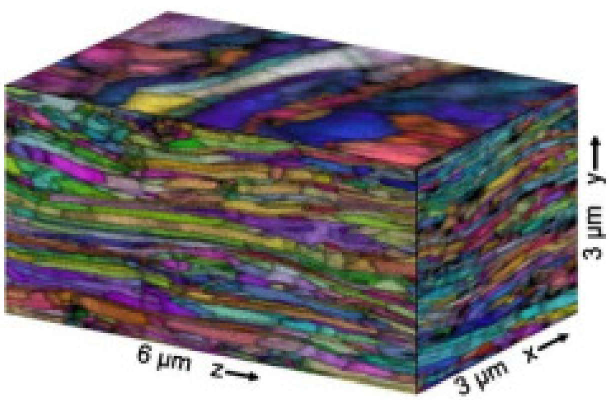
## Special properties

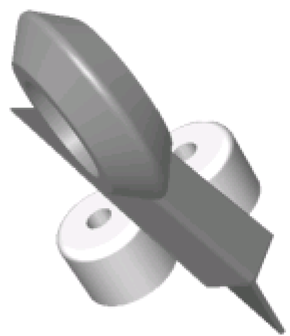
- Increased strength
- High wear resistance
- Superplasticity

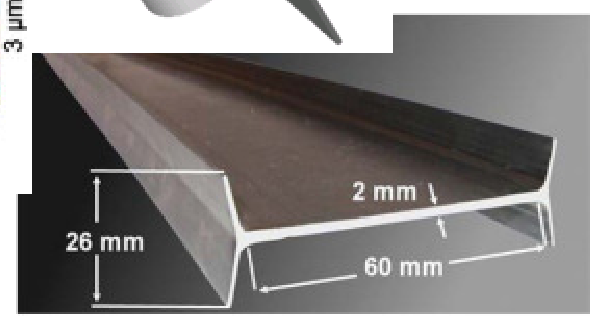
Ductility ⟷ Strength




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



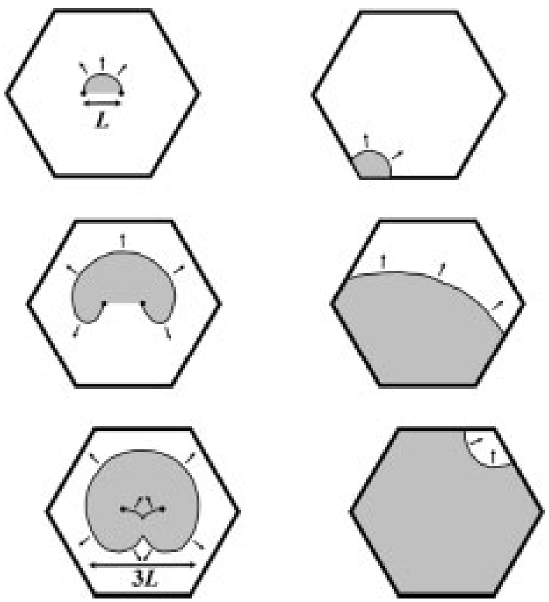



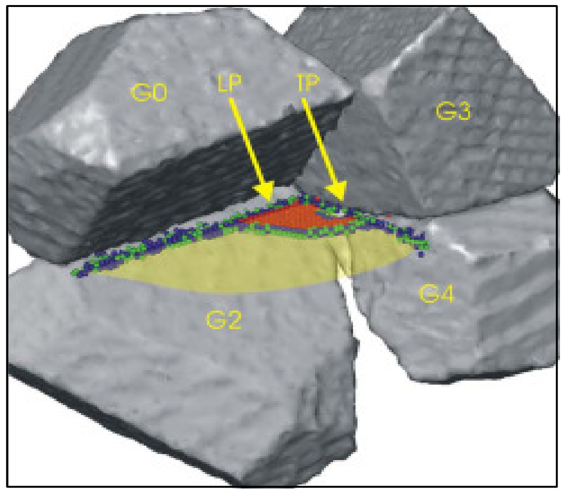



Linear Flow Splitting

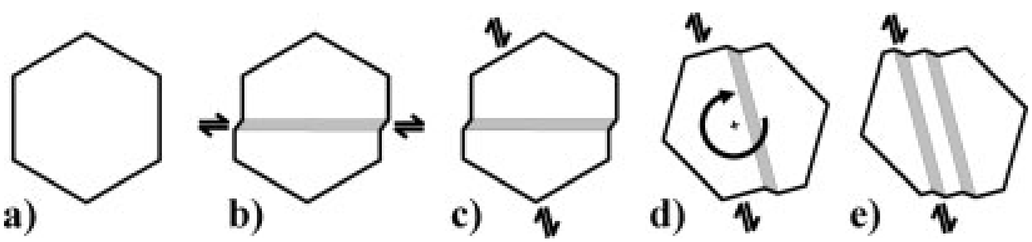
Bohn et al., J Mater Sci 43 (2008) 7307

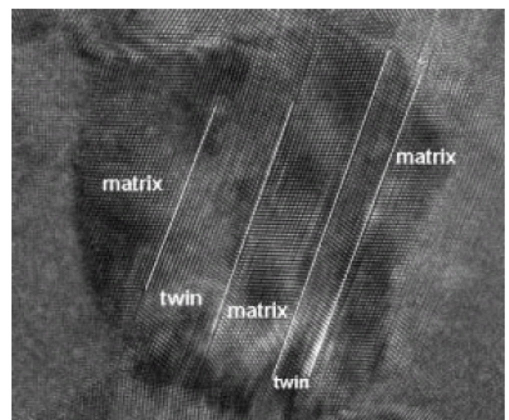
# nc-Metals: Insights and Puzzles




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



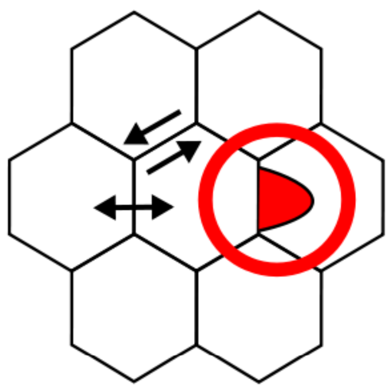




H. Rösner, J. Markmann, J. Weissmüller, *Philos. Mag. Lett.* **2004**, *84*, 321.

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

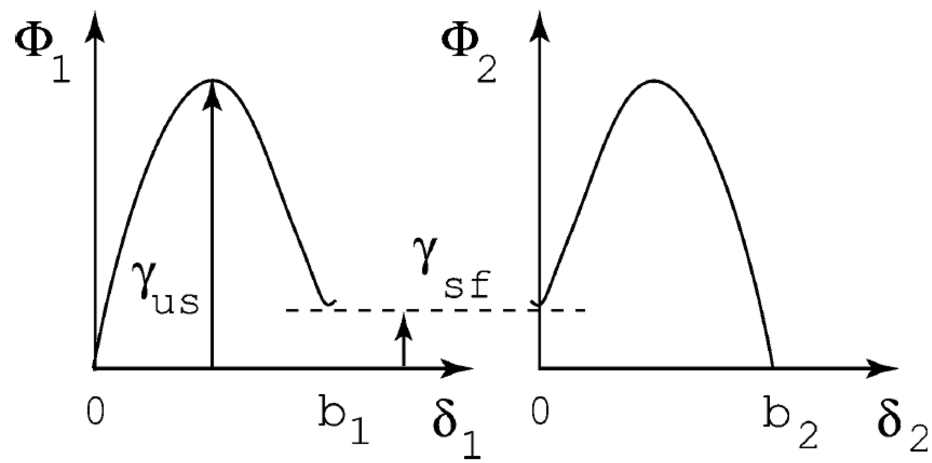
# Dislocation nucleation



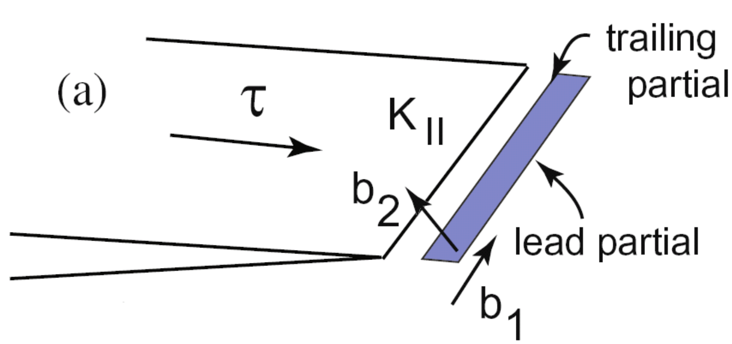


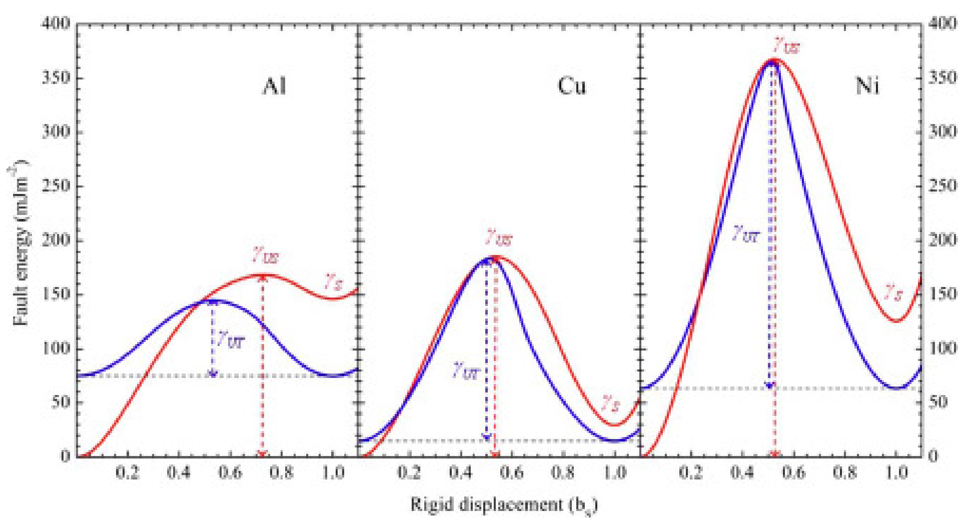
$R = (\gamma_{usf})/Gb$

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

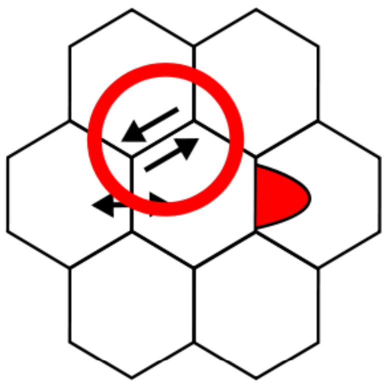


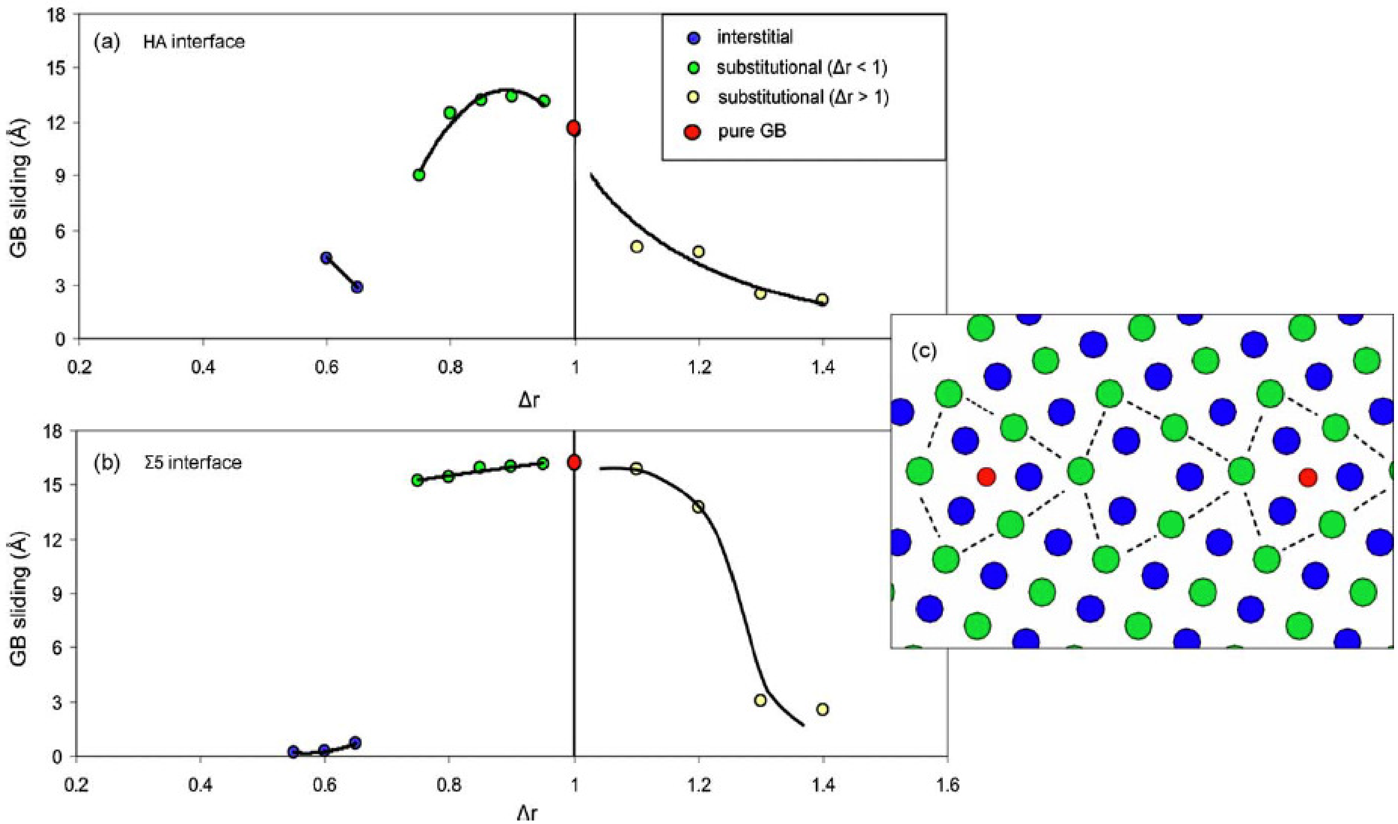

Asaro, Suresh, Acta Mater., 53 (2005)



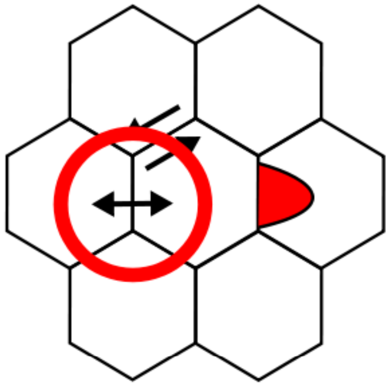
# GB sliding

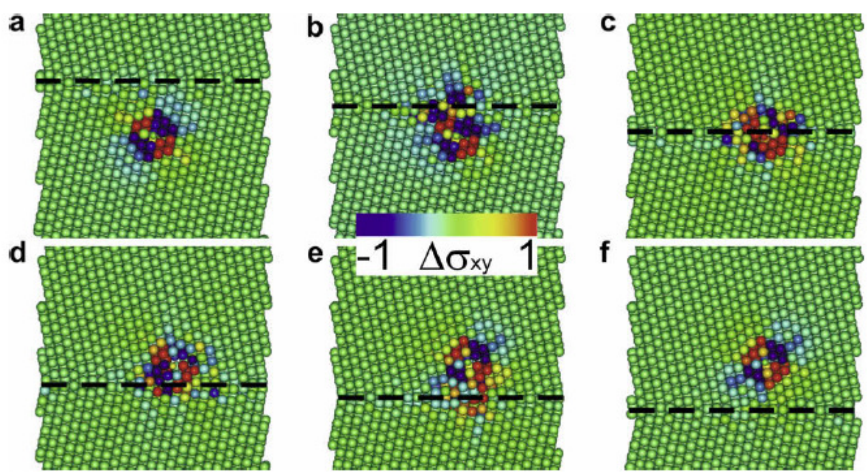


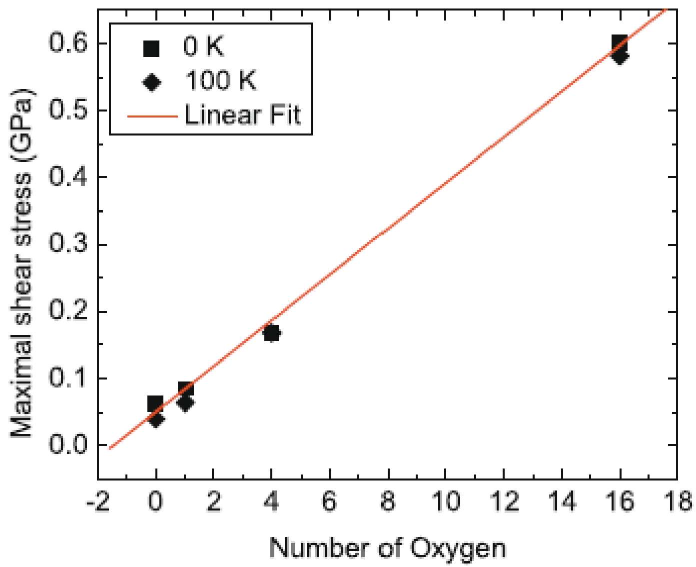



Millett et al., Mat. Sci. Eng. A, 431 (2006)

# Coupled GB motion






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

# Thermal Activation: Stress Exponent



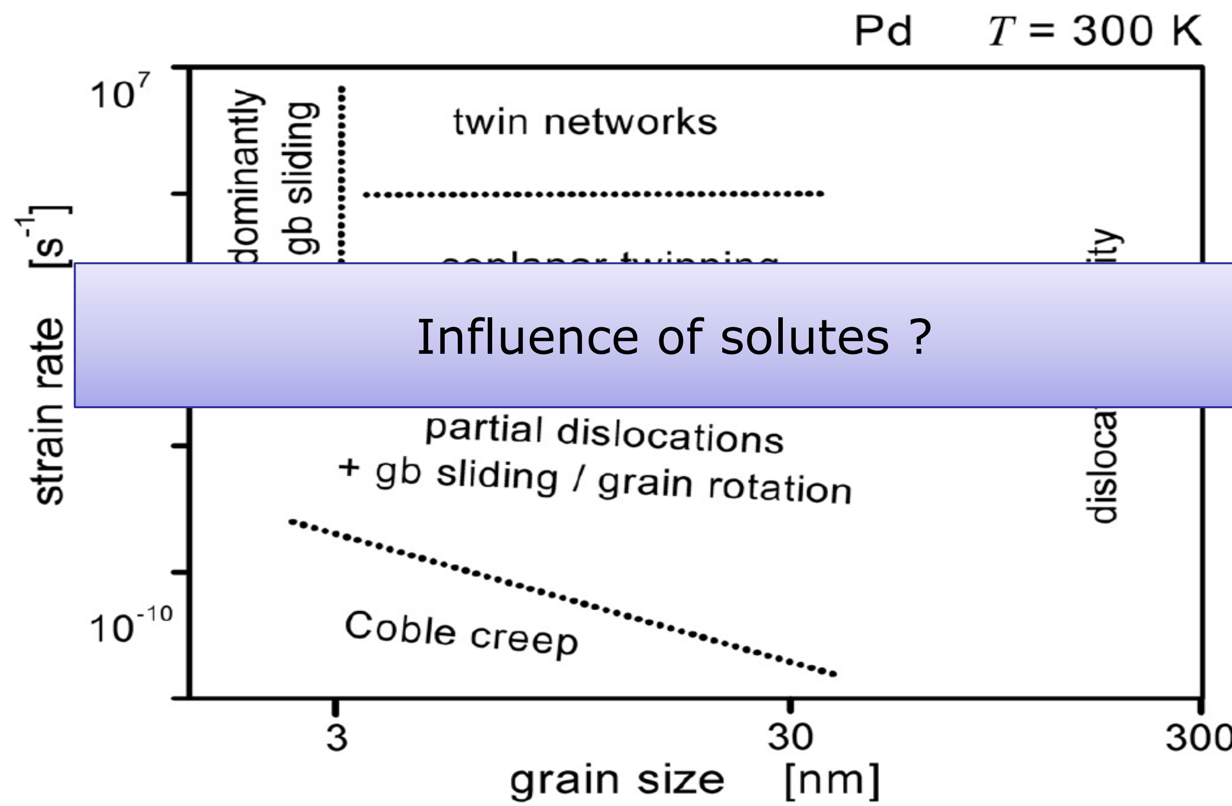
Orowan−Eq: $\dot{\gamma} = \rho b\langle v\rangle = \rho b\bar{l}\nu = \rho b l \nu_o e^{-\frac{\Delta G^*(\tau^*)}{k_B T}}$

$$\dot{\gamma} = \dot{\gamma}_o e^{-\frac{\Delta G^*(\tau^*)}{k_B T}} \rightarrow -k_B T \ln\left(\frac{\dot{\gamma}}{\dot{\gamma}_o}\right) = \Delta G^* = \Delta F^* - \tau \Delta V^*$$

Activation Volume: $\Delta V^* = -\left(\frac{\partial \Delta G^*}{\partial \tau^*}\right)_T = \frac{k_B T}{\tau^* \left(\frac{\partial \ln \dot{\gamma}}{\partial \ln \tau^*}\right)_T}$

Stress Exponent: $m = \left(\frac{\partial \ln \dot{\gamma}}{\partial \ln \tau^*}\right)_T = \frac{k_B T}{\Delta V^* \tau^*}$

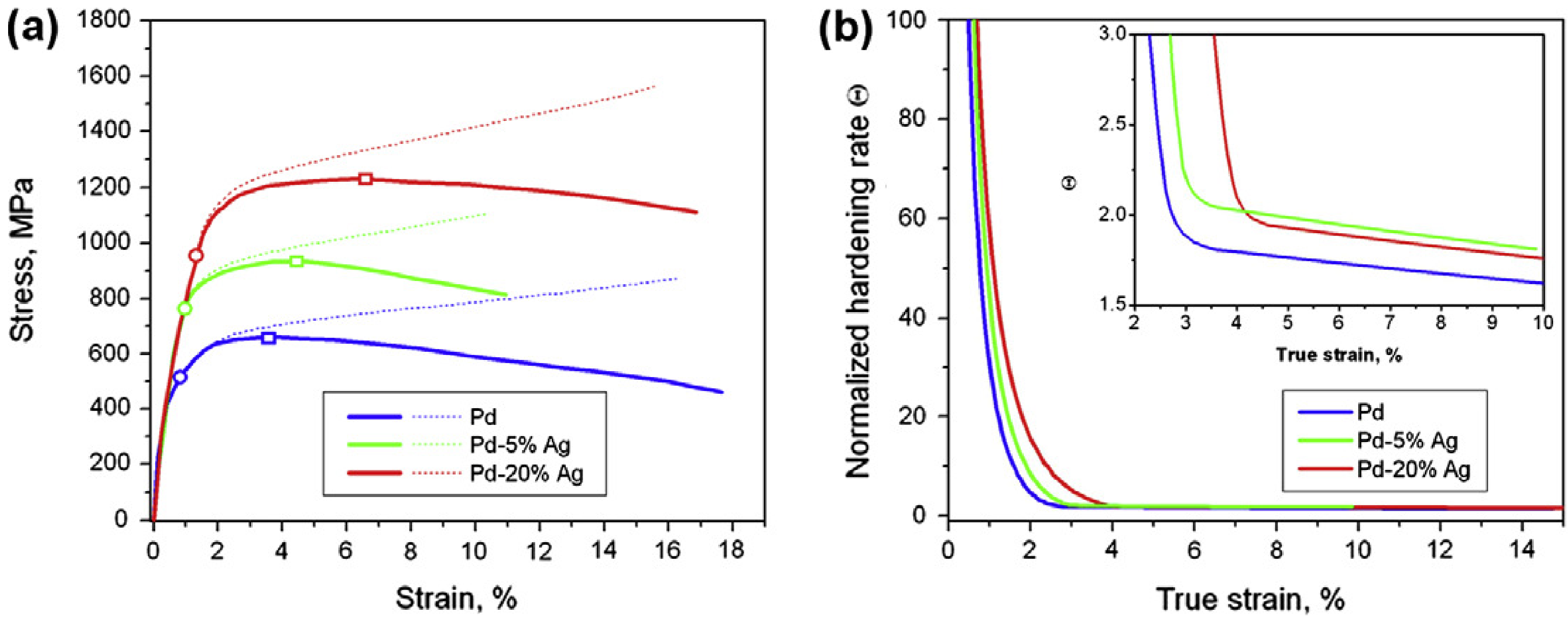
# nc-Metals: Insights and puzzles



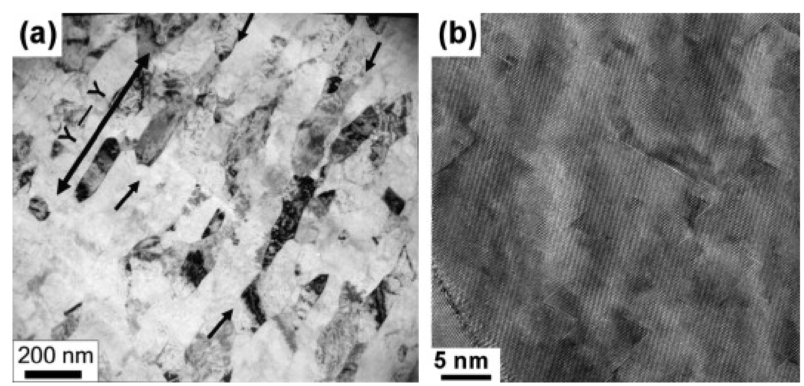

Influence of solutes ?

Weissmüller and Markmann, Advanced Engineering Materials, 202, 7 (2005)

# Nanocrystalline Pd-Au: Experiments




K. Yang et al., Acta Materialia 58 (2010) 967–978



# Modelling plasticity in nc alloys

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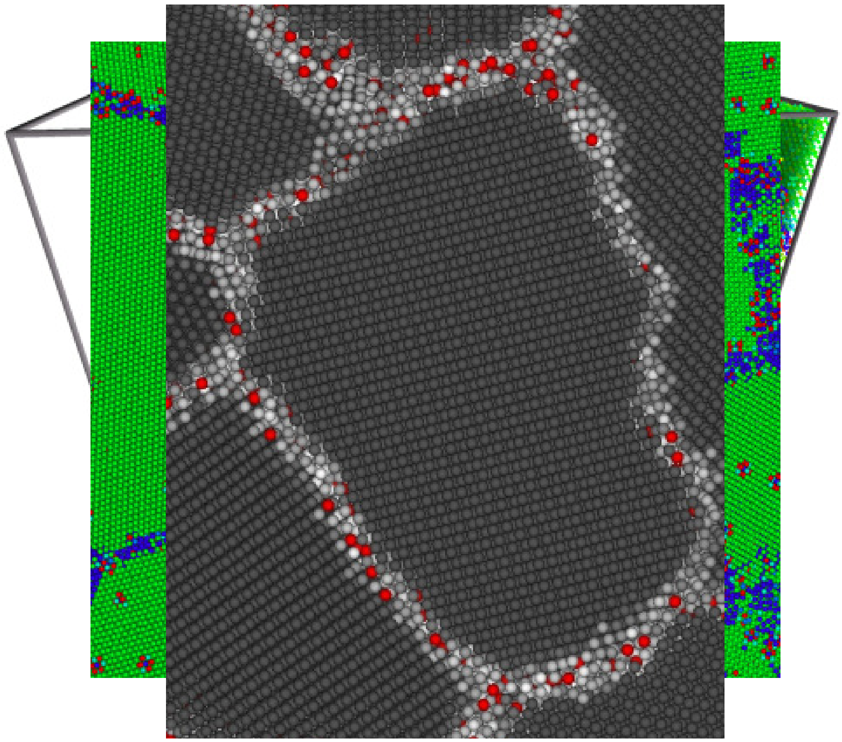
| | |
|---|---|
| Structure creation | Voronoi tesselation method |
| Grain size | 5 to 15 nm |
| Annealing | Hybrid MD/MC method |
| miscible | PdAu |
| | |
| segregating | Cu + X<br>X = Nb, Fe, Ag |



# Variance constrained semi-grandcanonical scheme

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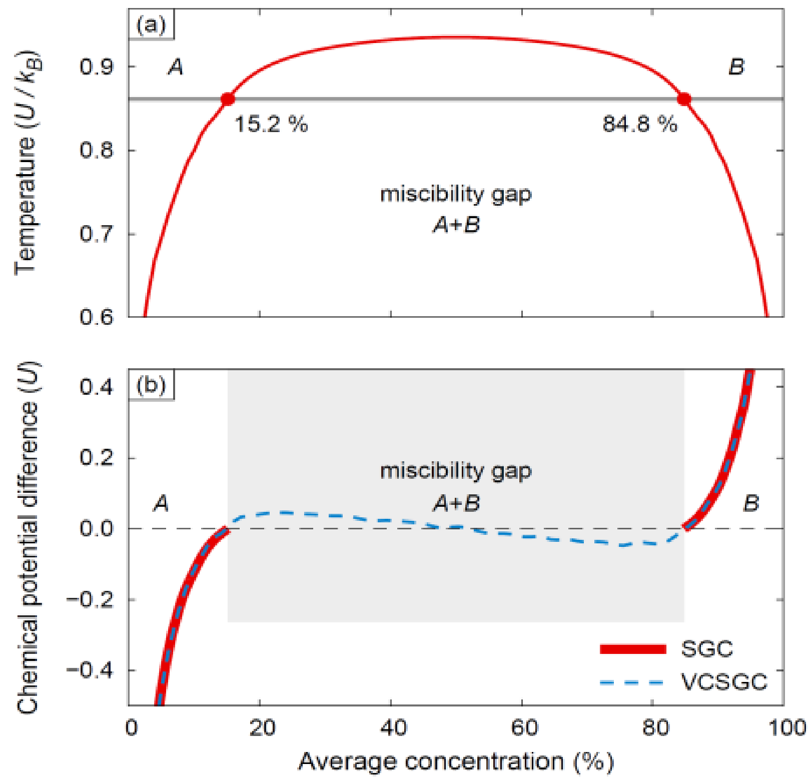
- The VCSGC-MC method imposes a constraint on the variance of the concentration, and allows for equilibration at arbitrary global concentrations.

- It allows to model the equilibrium properties of phase segregated multicomponent systems containing millions of particles.




**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]

# Acceptance Probabilities



Canonical

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

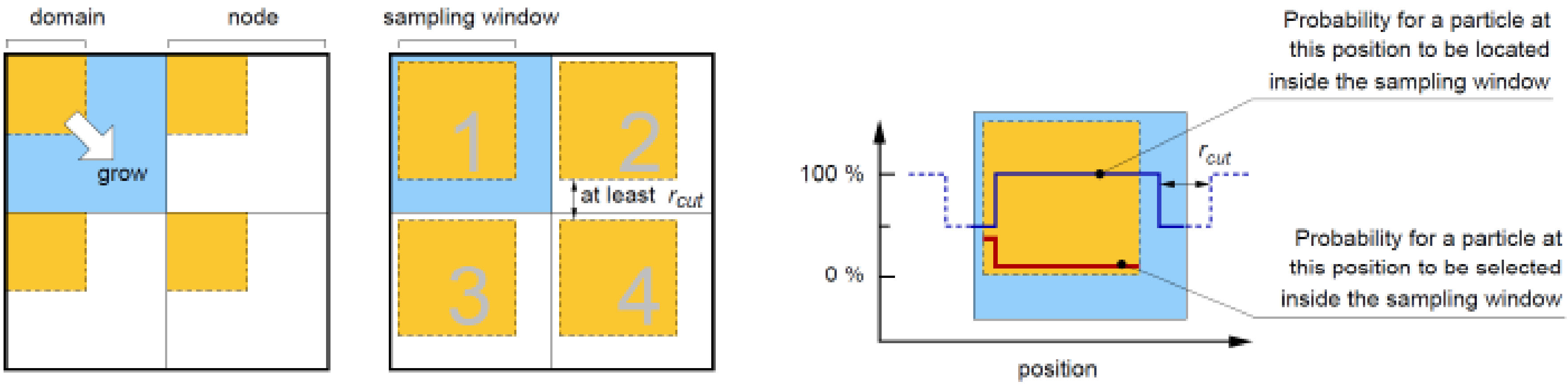
Semi-Grandcanonical

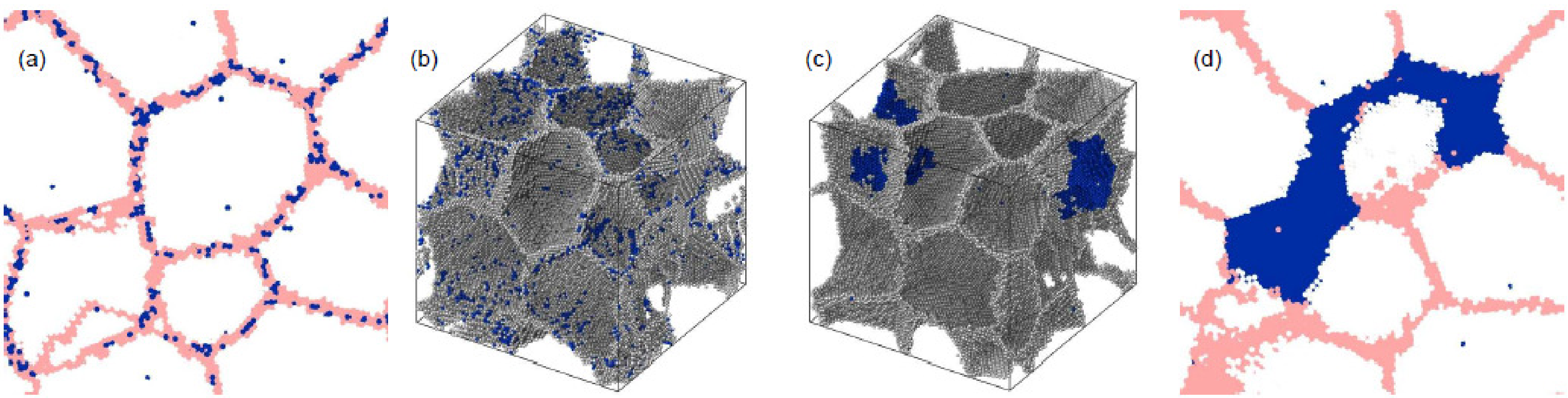
$$\mathcal{A}_{\mathrm{S}} = \min\left\{1, \exp\left[-\beta(\Delta U + \Delta\mu N \Delta c)\right]\right\}$$

Variance Constrained Semi-Grandcanonical

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

# Variance constrained semi-grandcanonical scheme: *Parallelization*



# OVITO
# (Open Visualization Tool)

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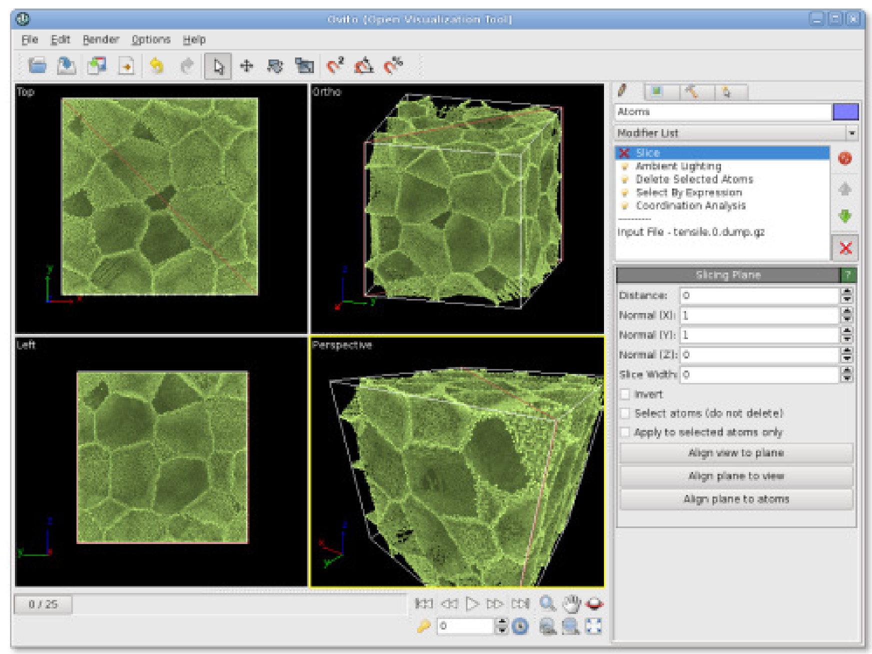
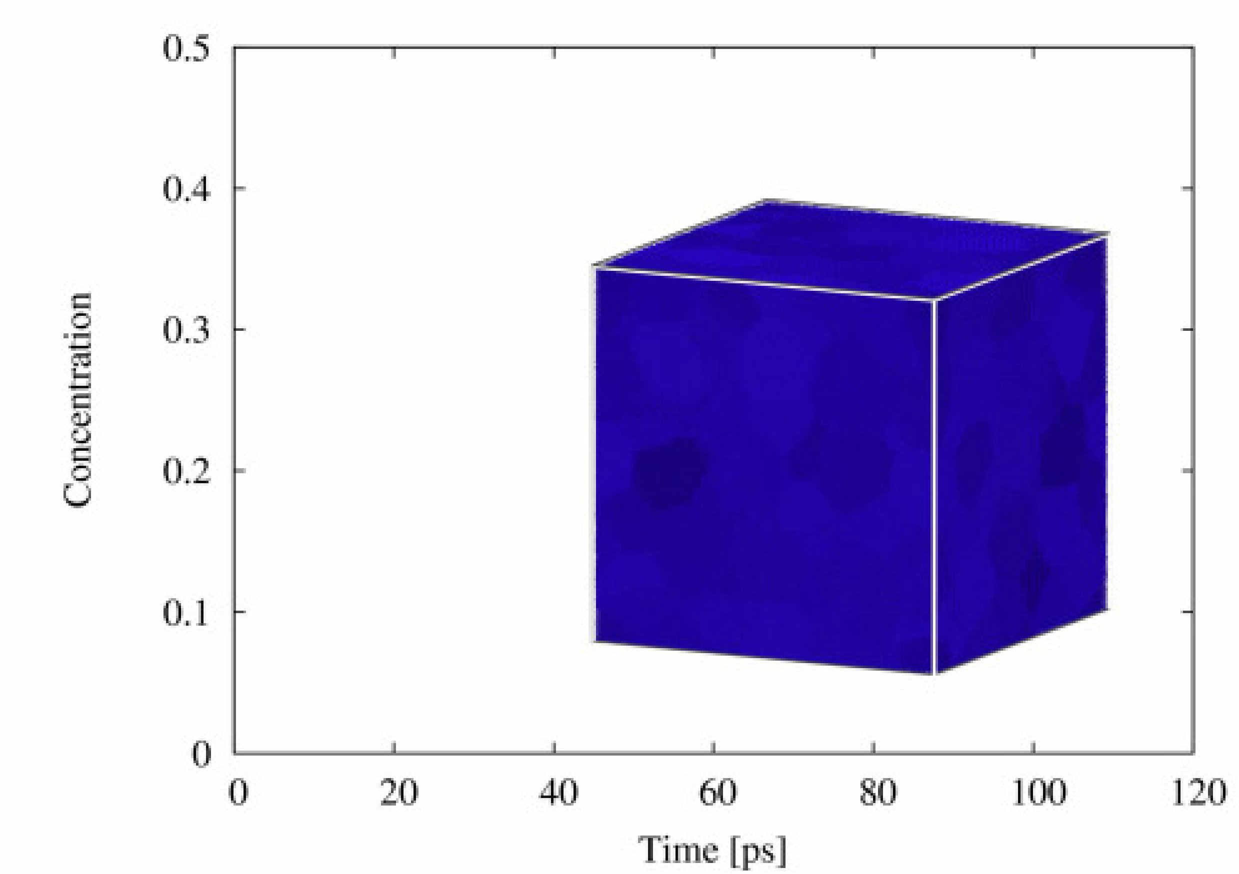
Visualization and analysis software for atomistic simulation data:

- 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)

# Annealing + Alloying: PdAu

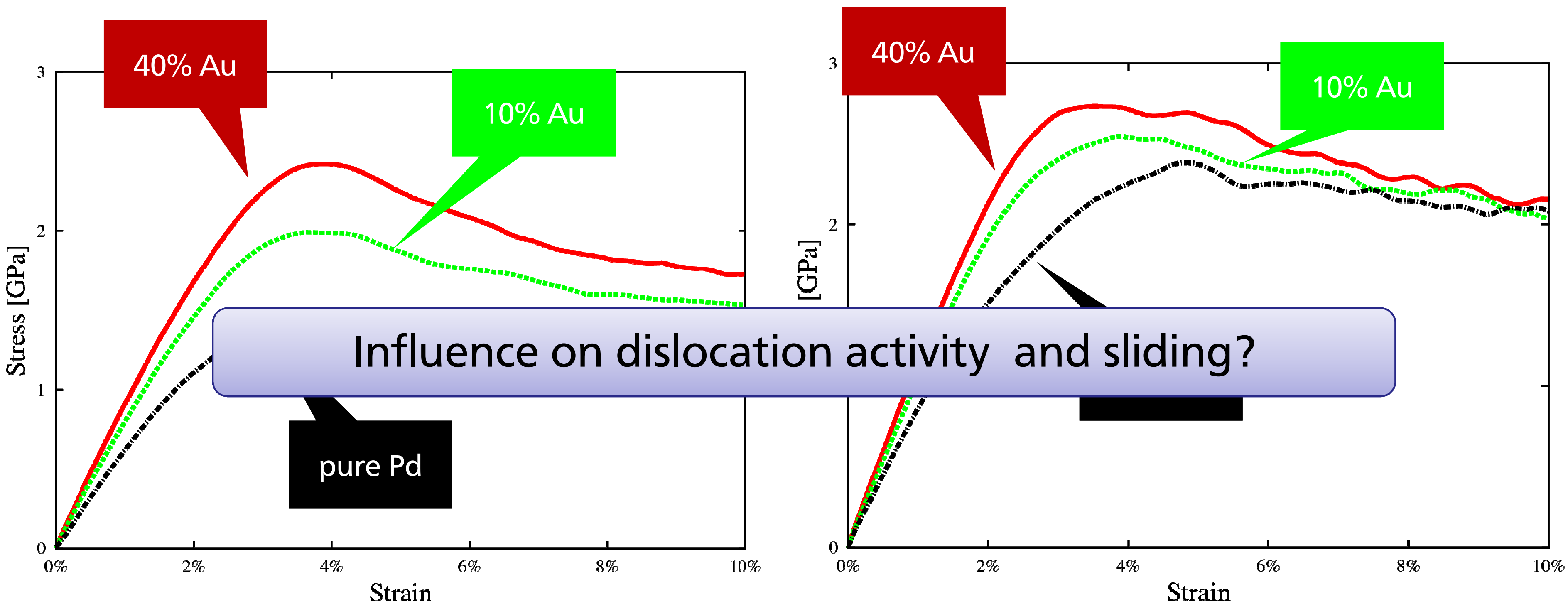



Grain

total

GB

# PdAu: Tensile straining: $\dot{\varepsilon}=10^8\ s^{-1}$; T=300K




5 nm

15 nm

# Dislocations extraction algorithm

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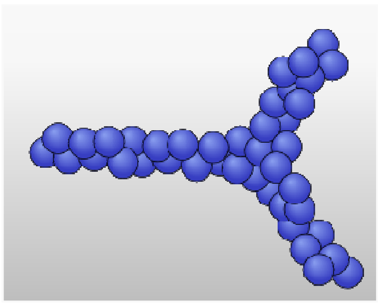
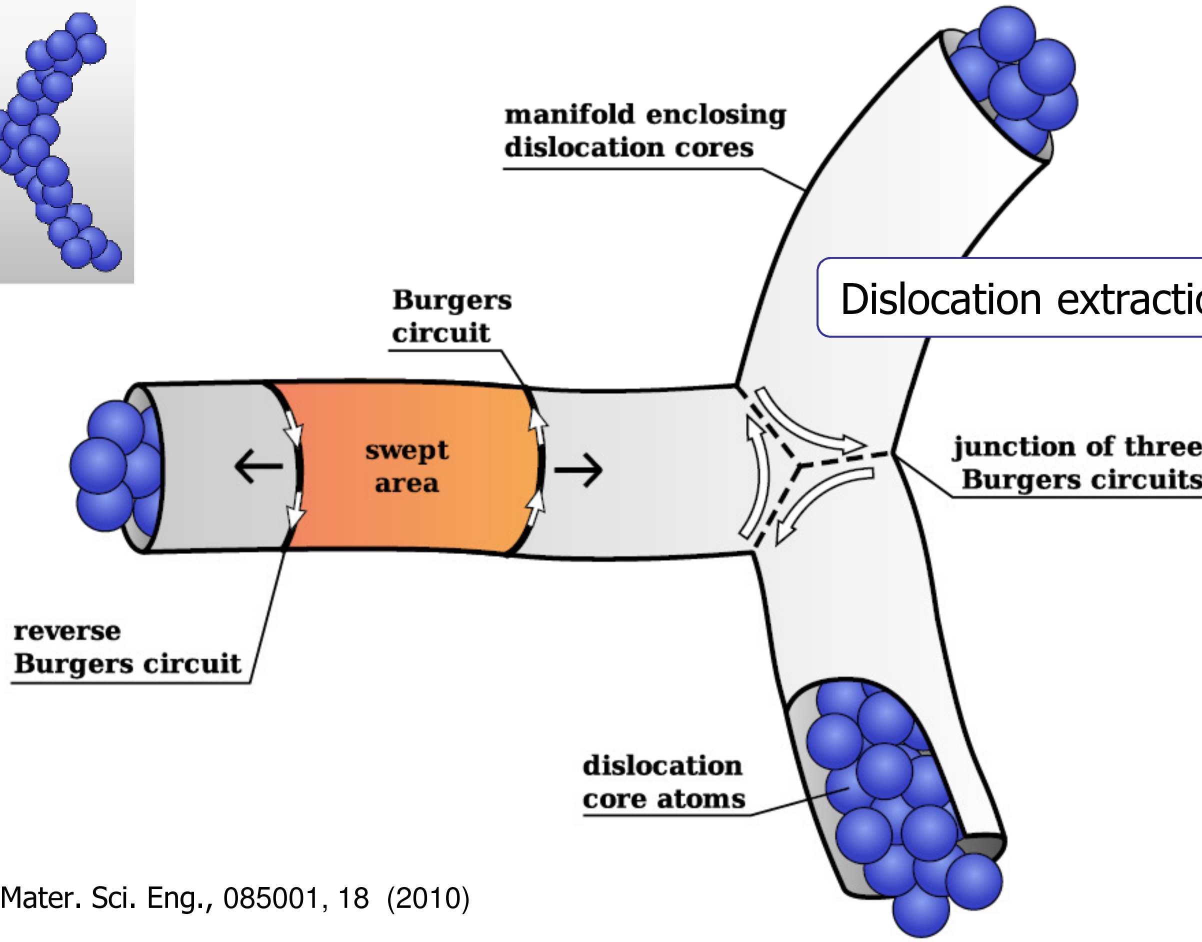
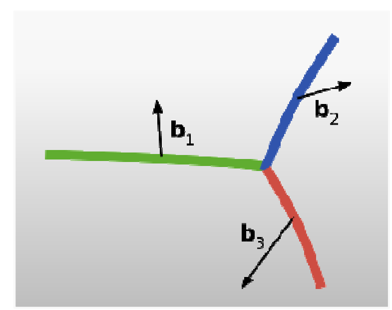




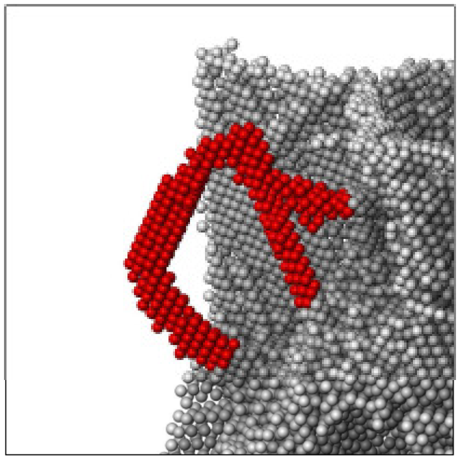

Dislocation extraction algorithm (DXA )

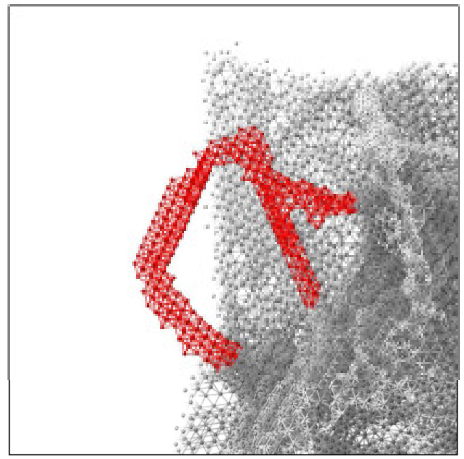


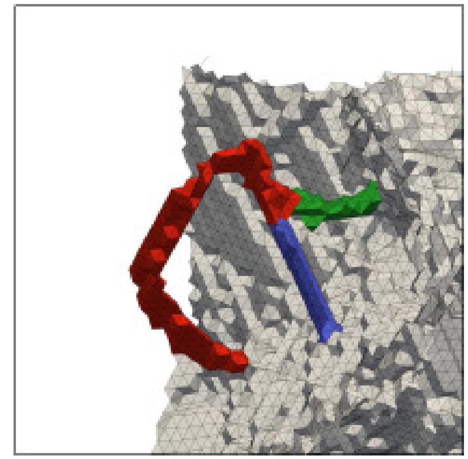

Modelling Simul. Mater. Sci. Eng., 085001, 18 (2010)

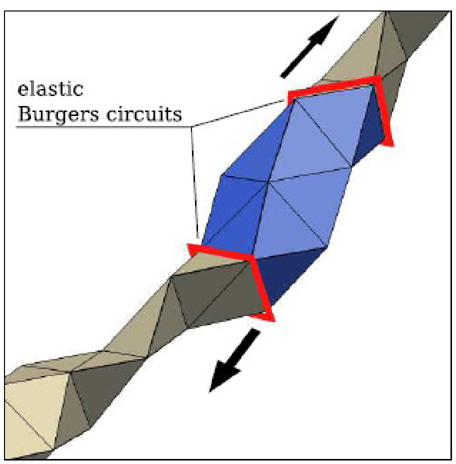
http://www.mm.mw.tu-darmstadt.de/~stuko/DXA/index.html

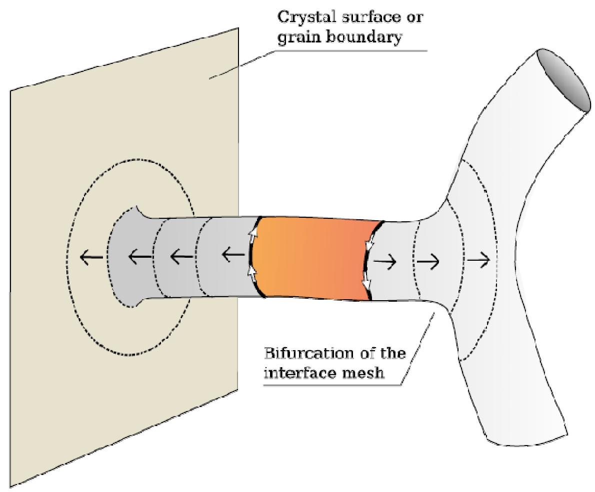
# Dislocation extraction algorithm

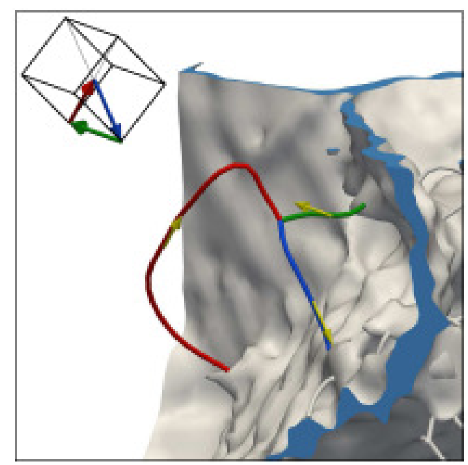








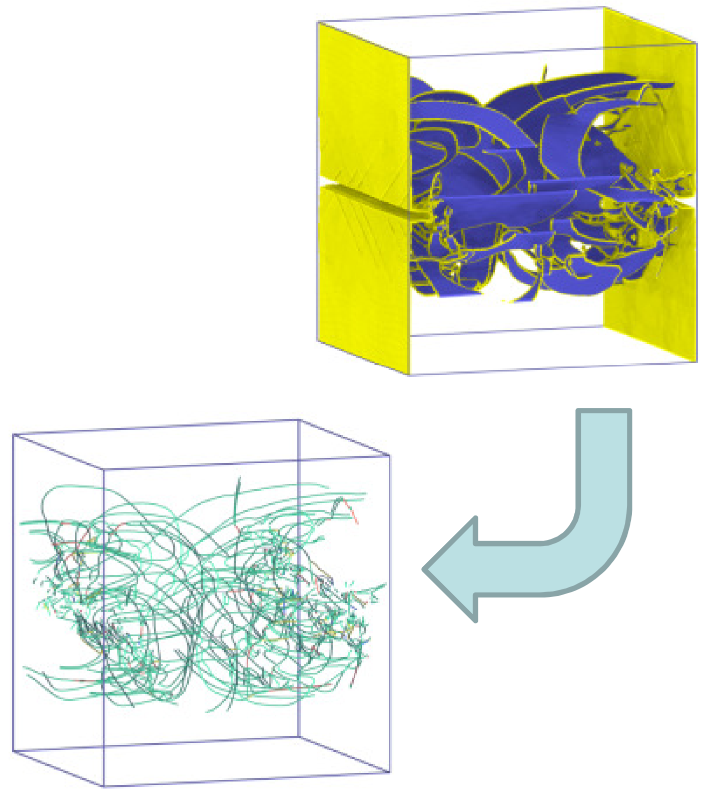



# Automated dislocation detection

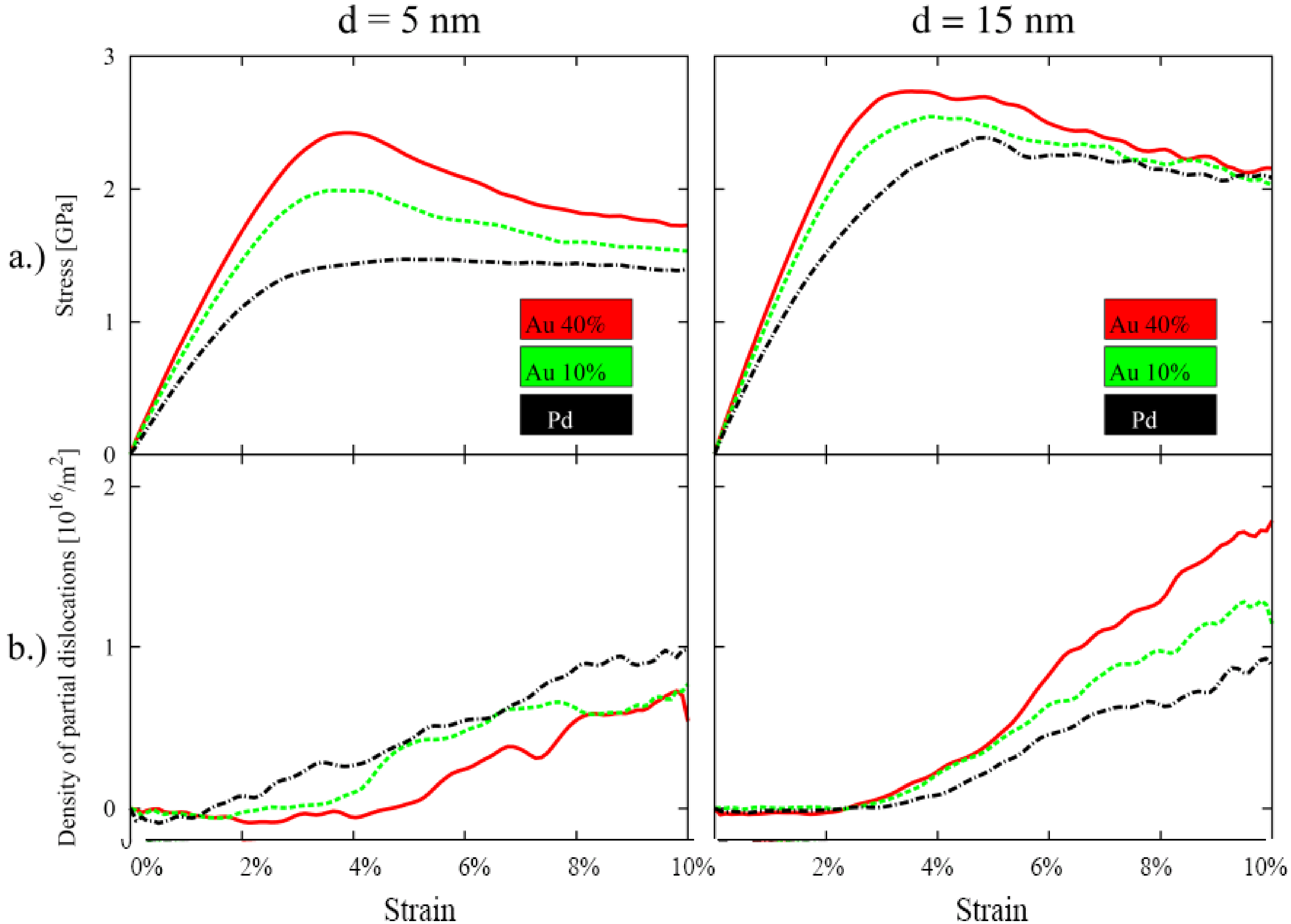


## What can we do with it?

- 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)

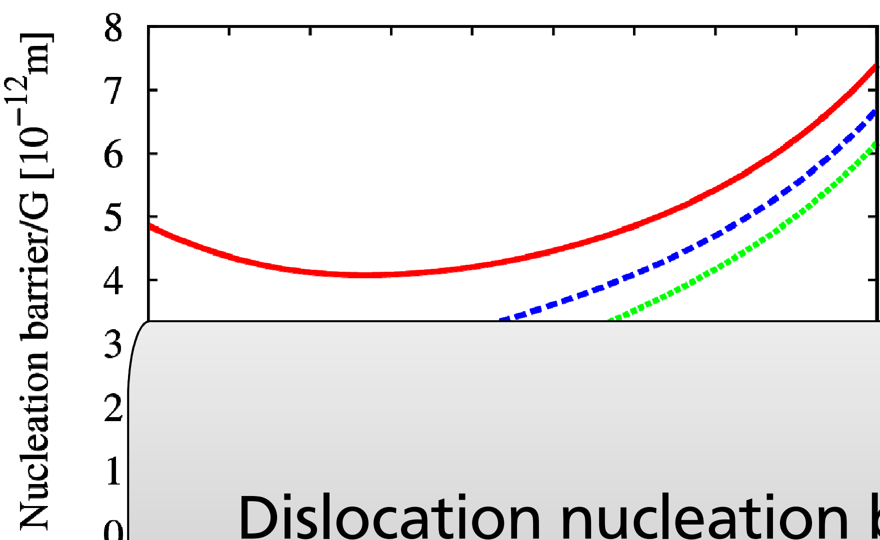


# PdAu: Tensile straining, $\dot{\varepsilon}=10^8\ s^{-1}$; T=300K

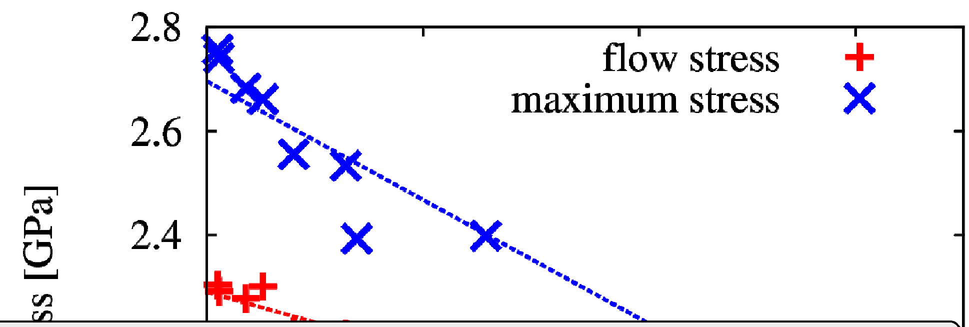


# PdAu: alloying effects

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




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

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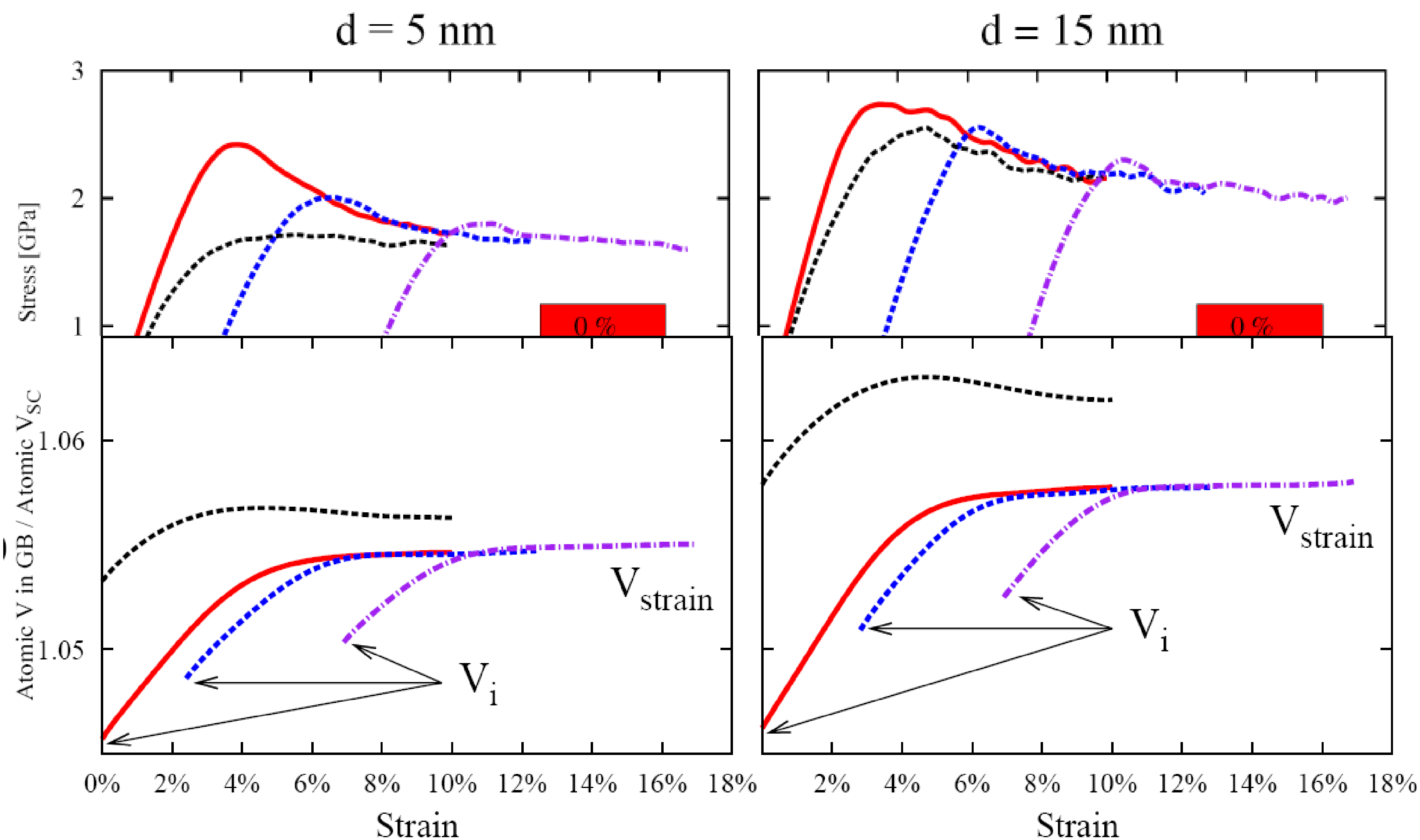

# PdAu: equilibration effects

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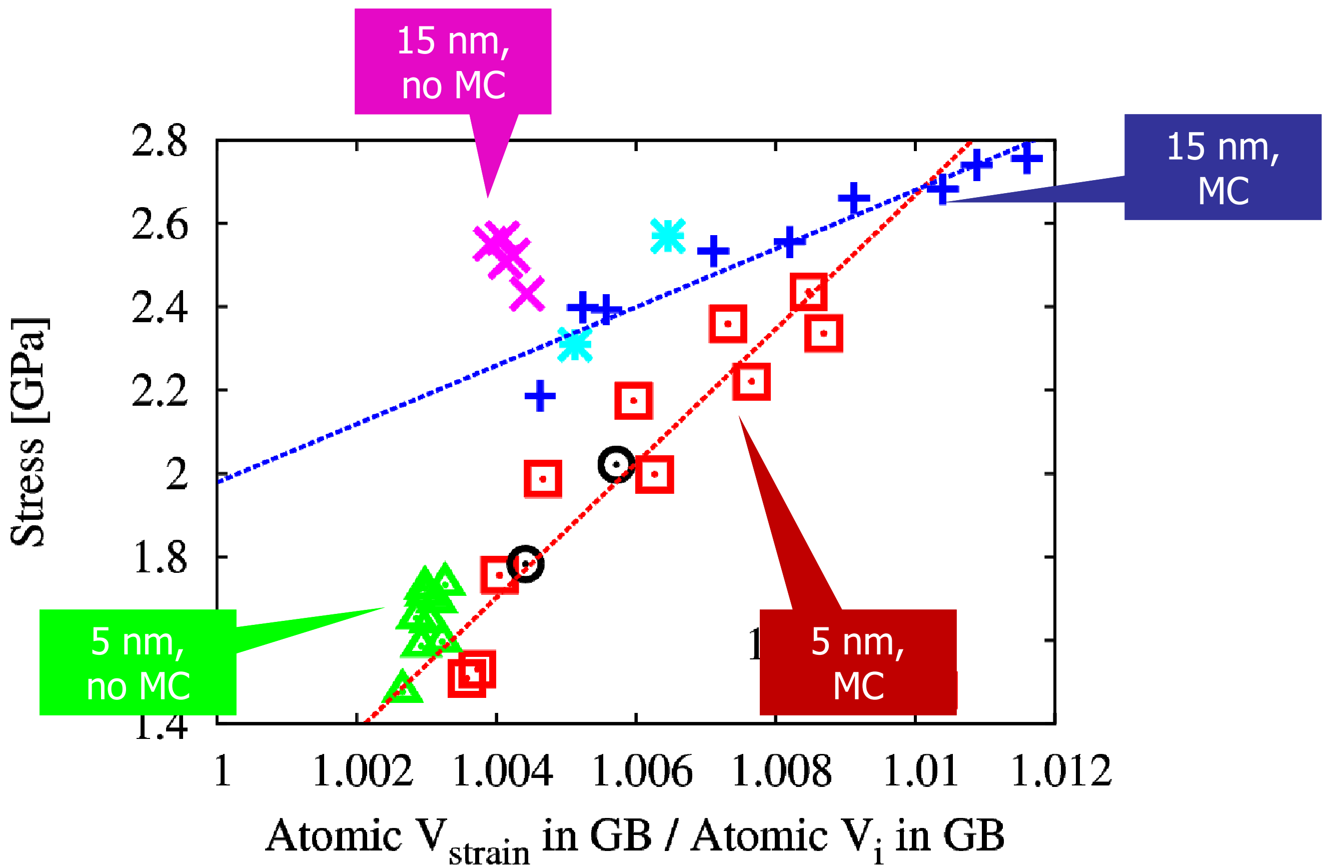
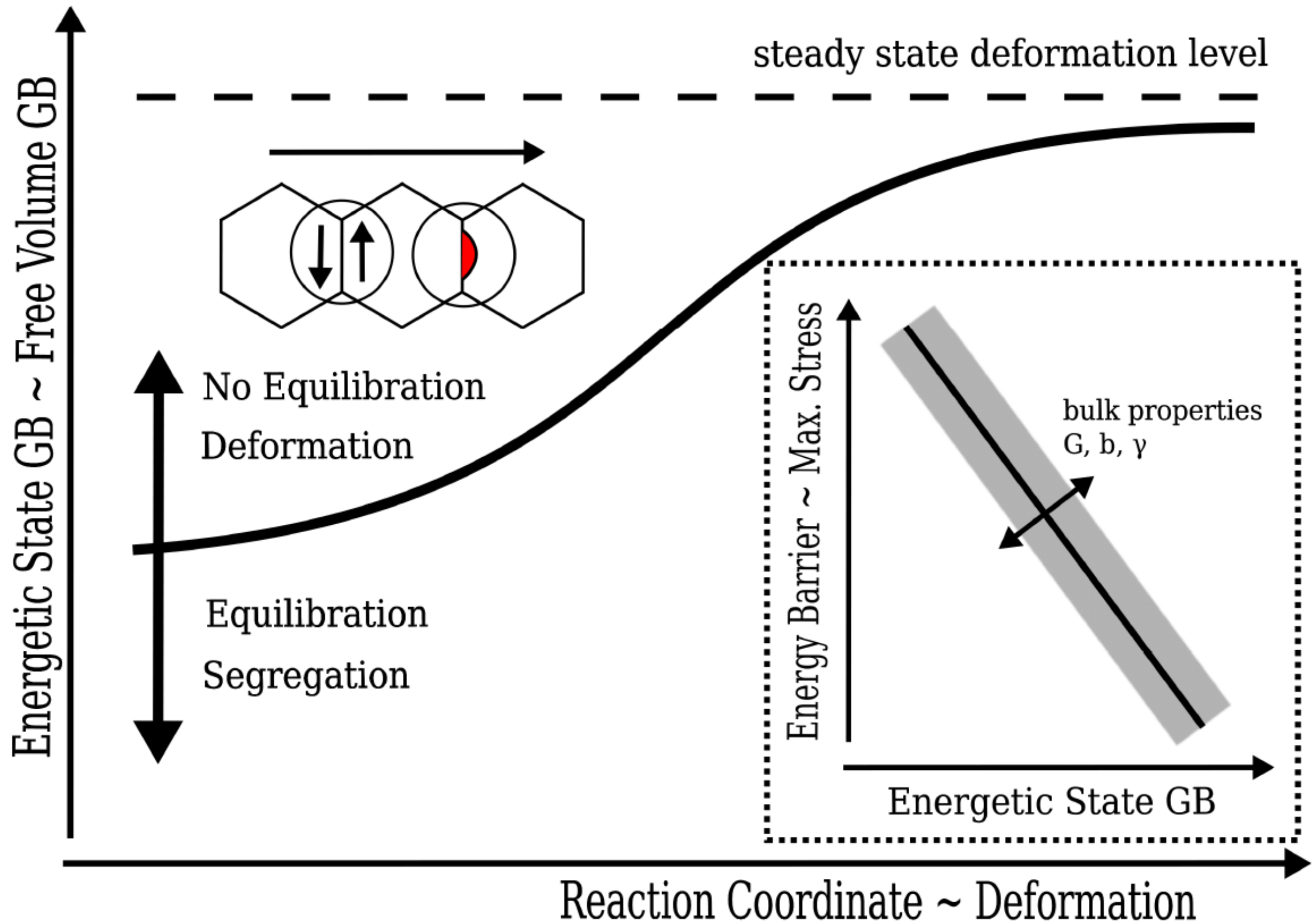
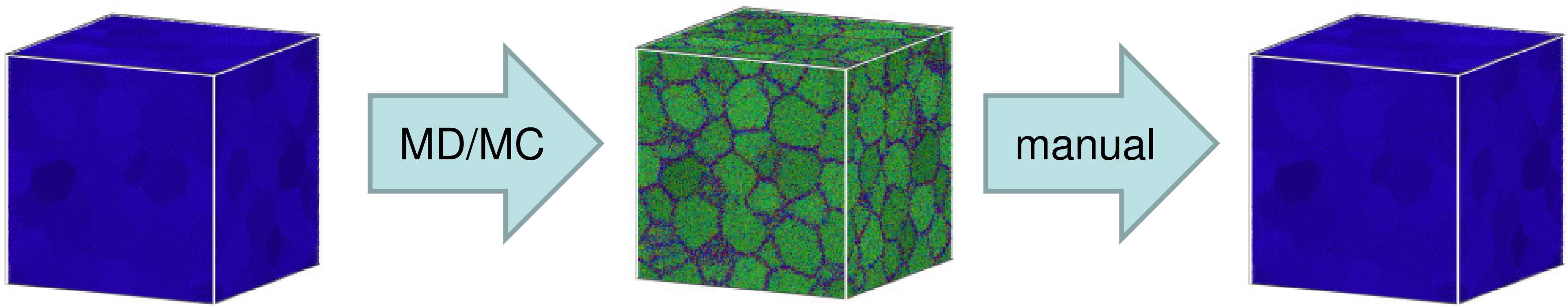


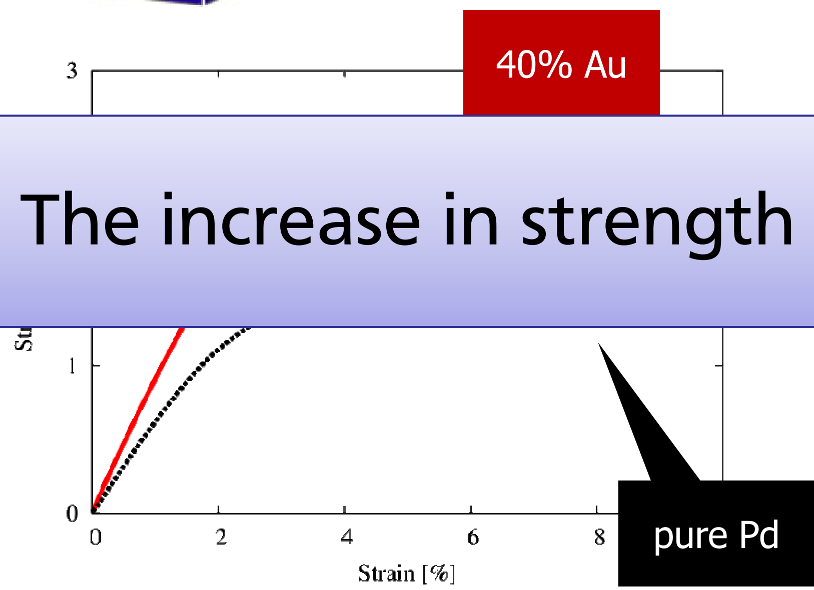

Schäfer et al., Acta Materialia, 59, (2011)

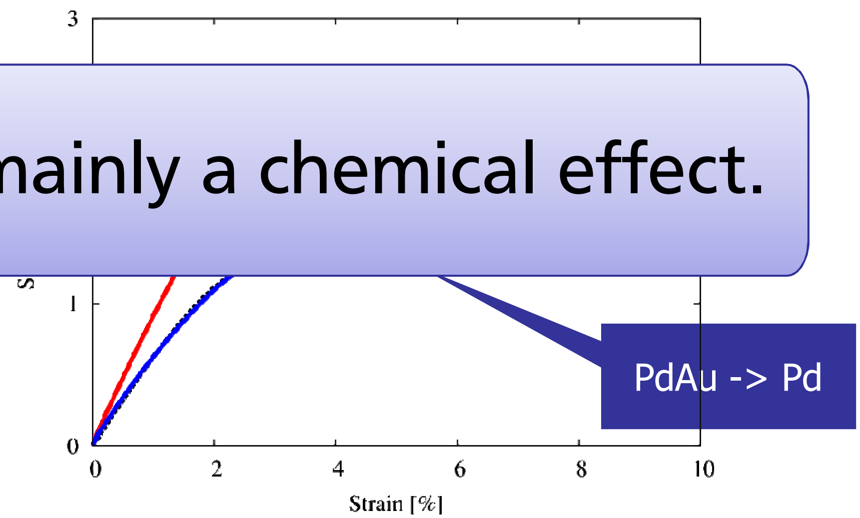
# „Steady-State“ of GB ?



# PdAu: Equilibration effects ?




The increase in strength is mainly a chemical effect.

# Deformation mechanisms:
# Variation of GB composition?

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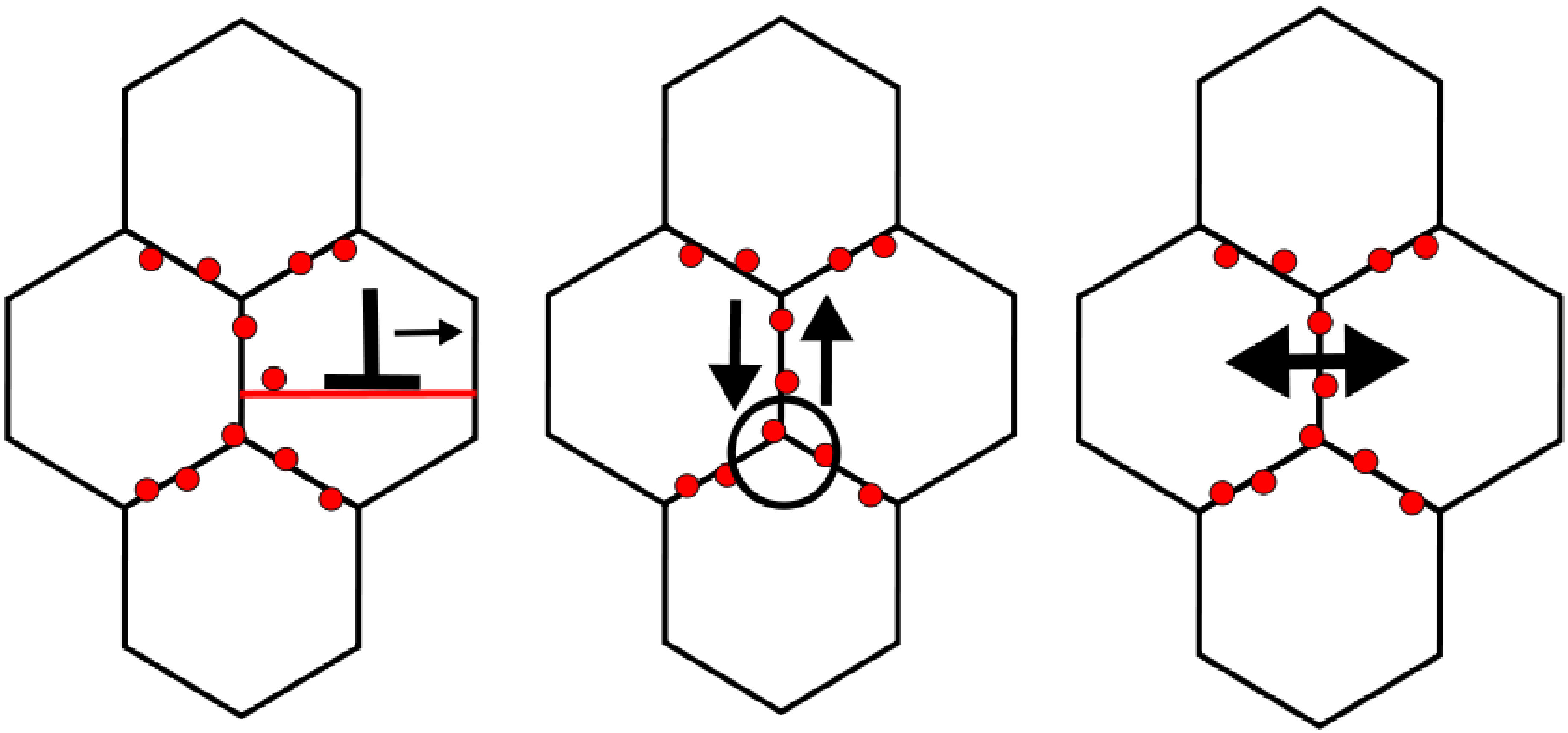
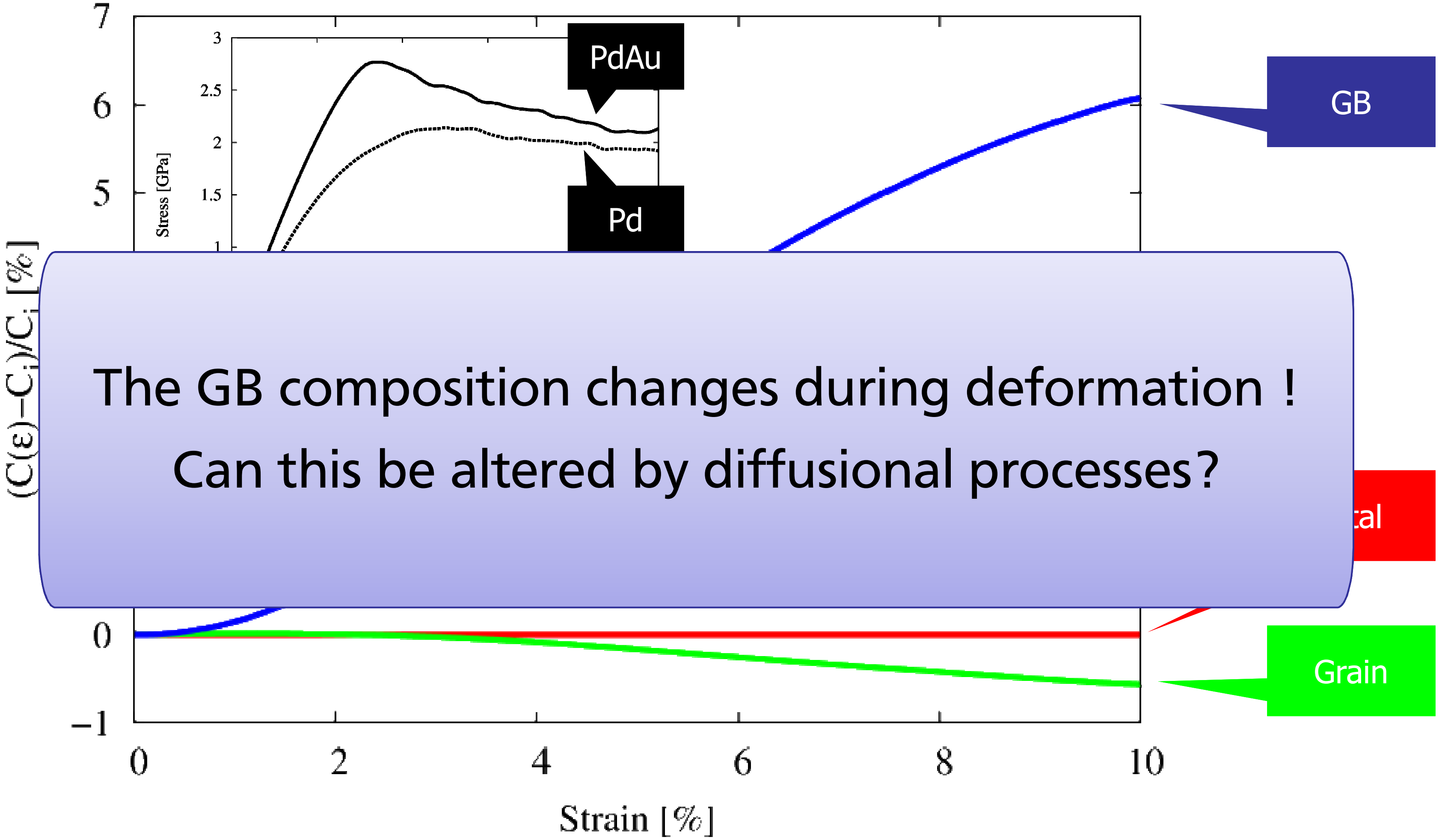


# GB composition during straining

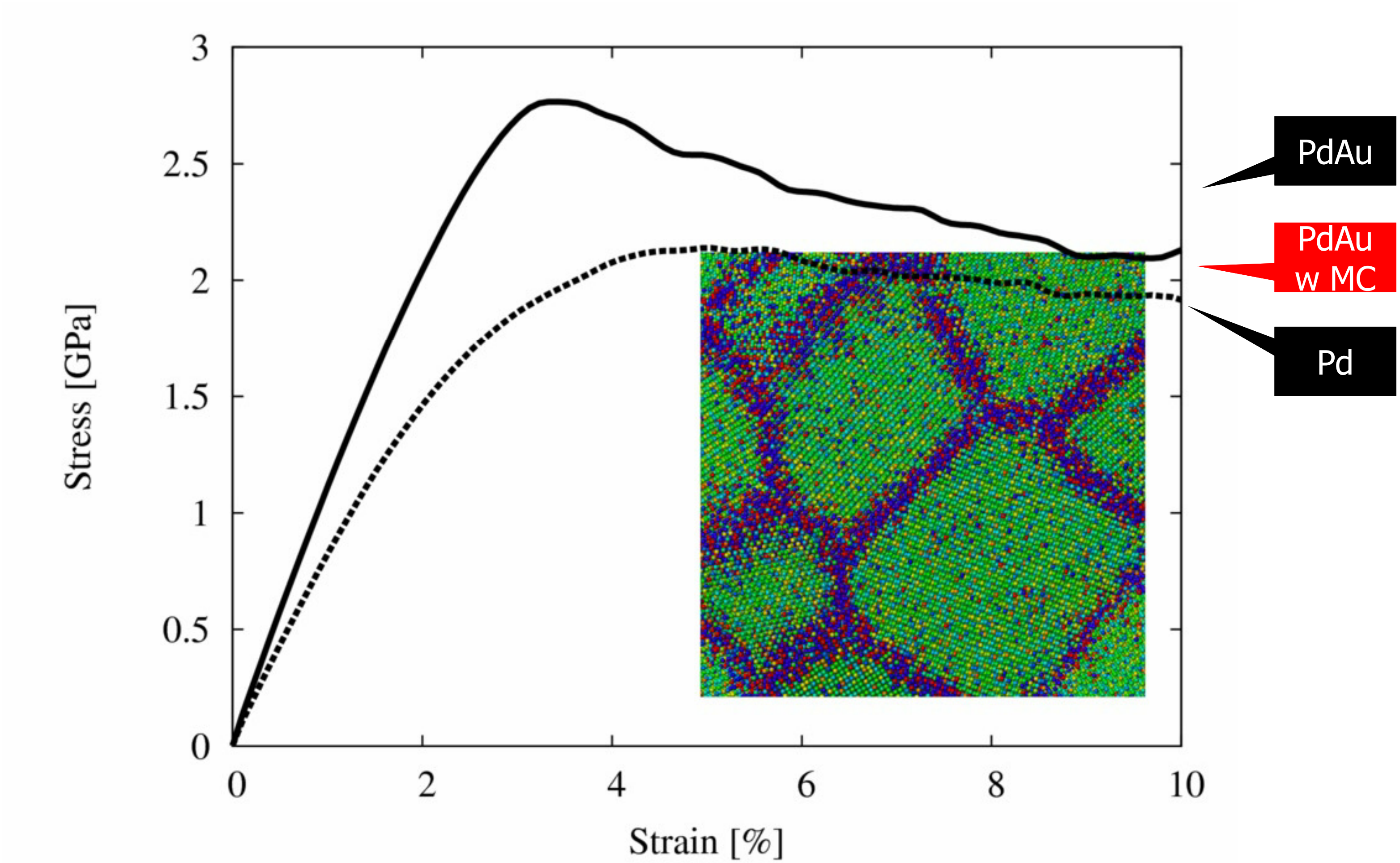



The GB composition changes during deformation !

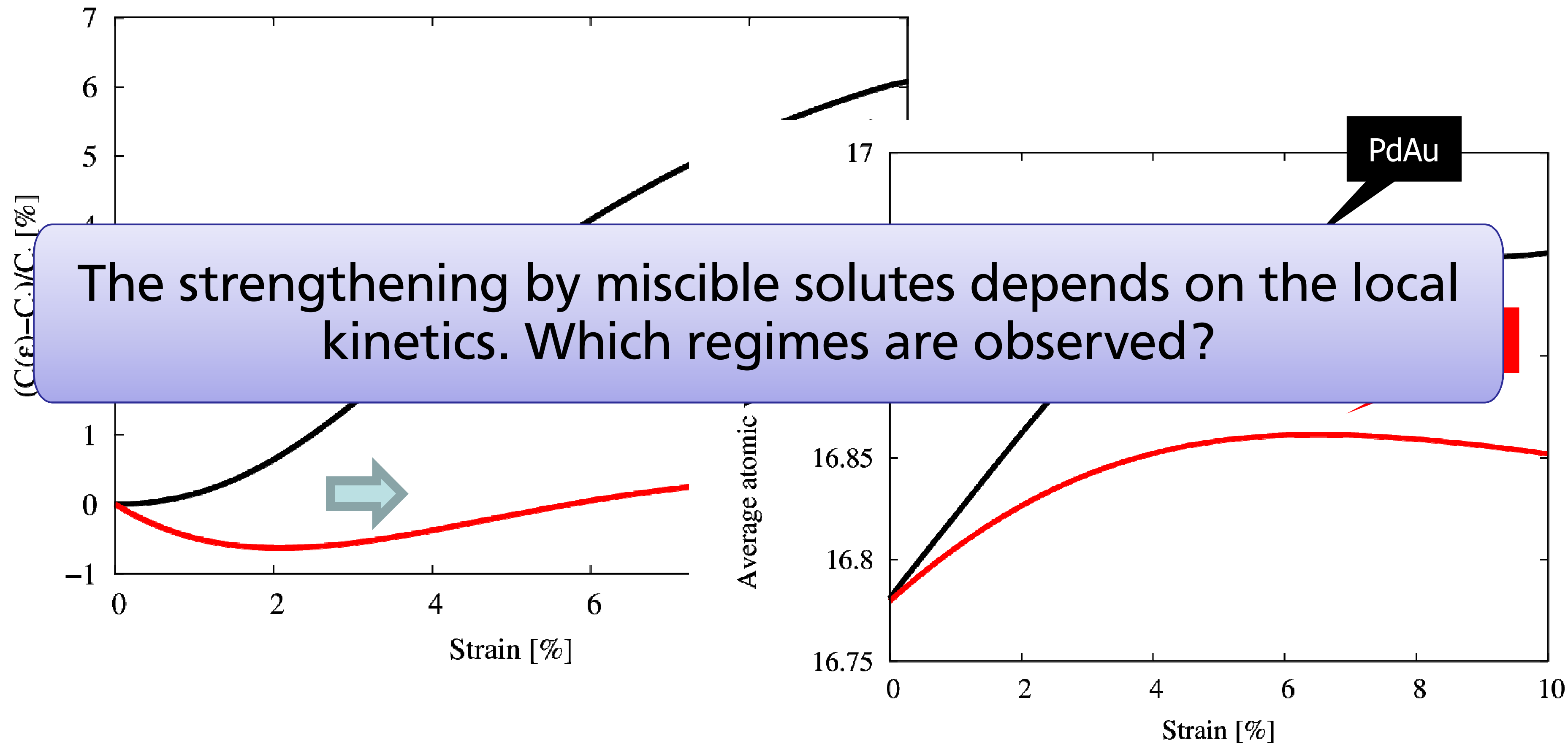
Can this be altered by diffusional processes?

# Shortcutting Diffusion





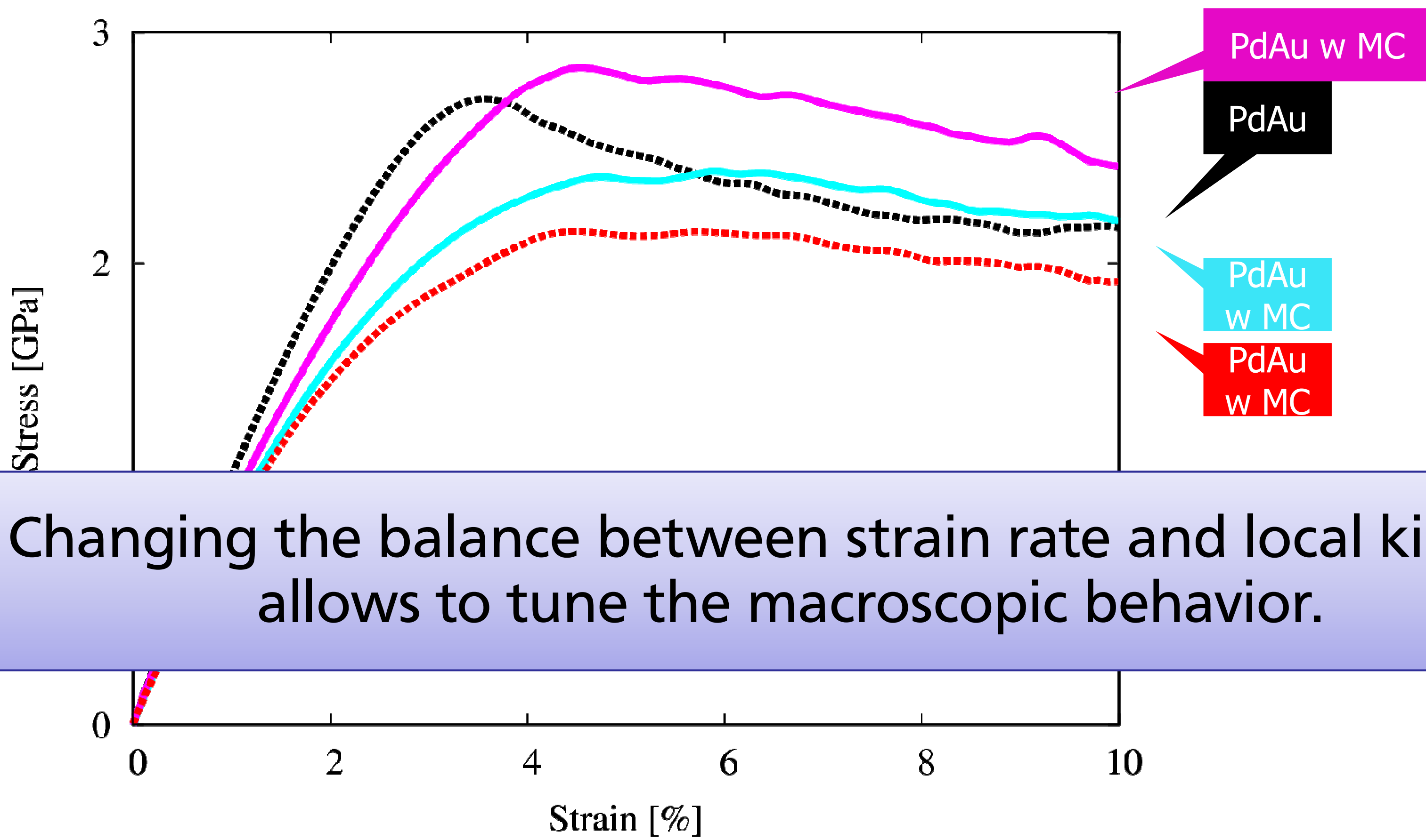
# Shortcutting Diffusion




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

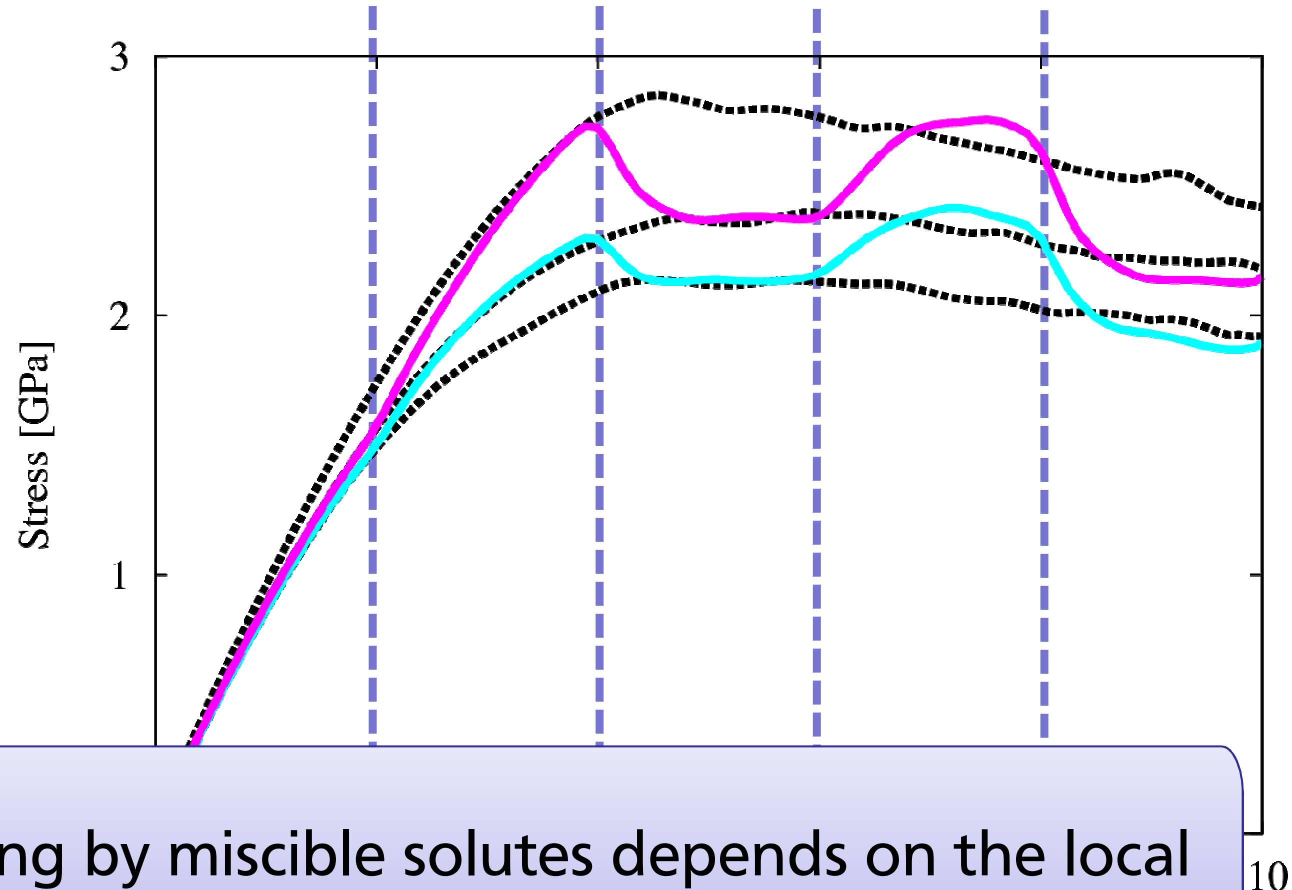
# Altering the Balance: 300 K, $\dot{\varepsilon}=10^8\ s^{-1}$






Changing the balance between strain rate and local kinetics allows to tune the macroscopic behavior.

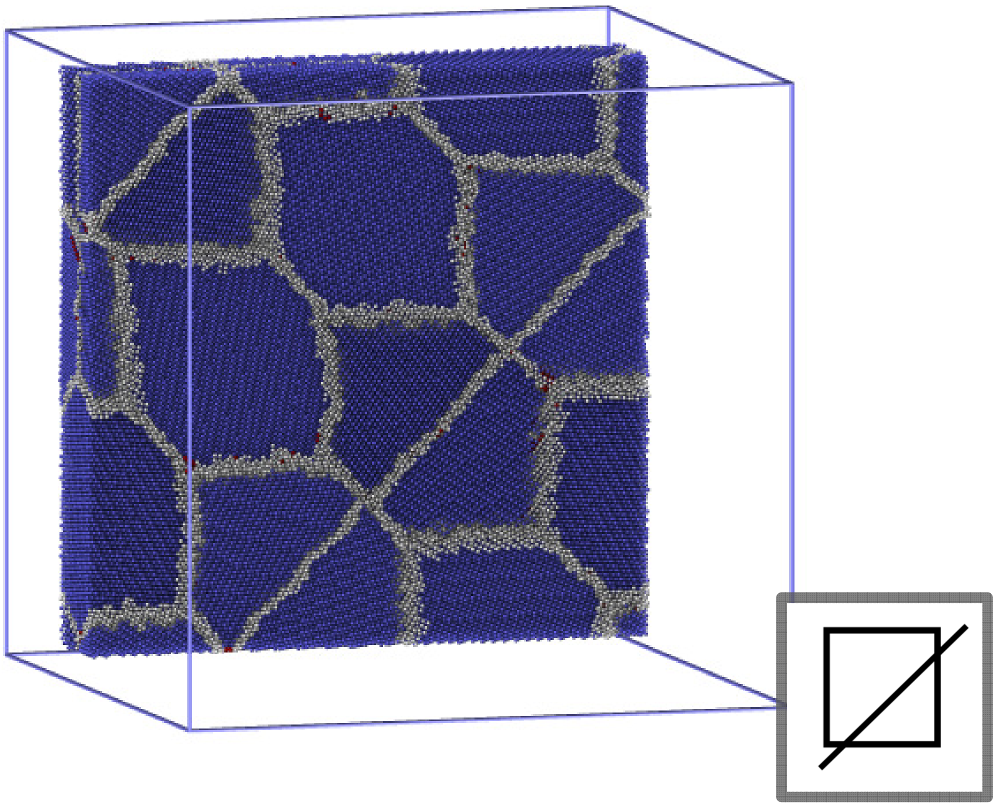
# Jump tests



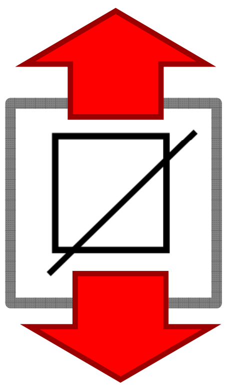

The strengthening by miscible solutes depends on the local kinetics. Can this be studied for individual mechanisms?

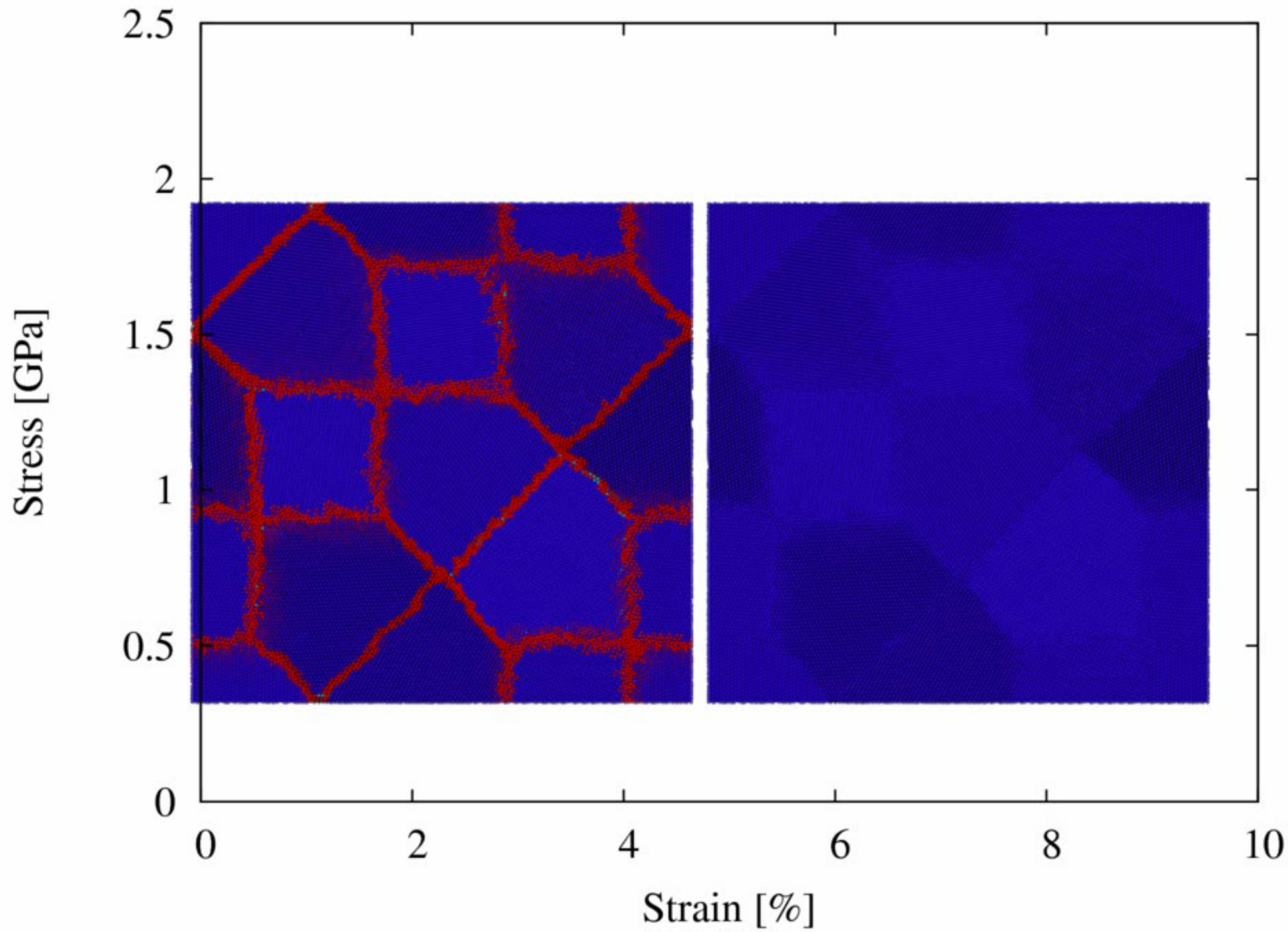
# Coupled Motion vs. Sliding

Subset of grain boundaries aligned

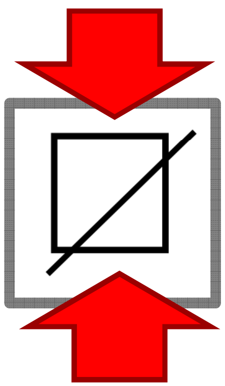


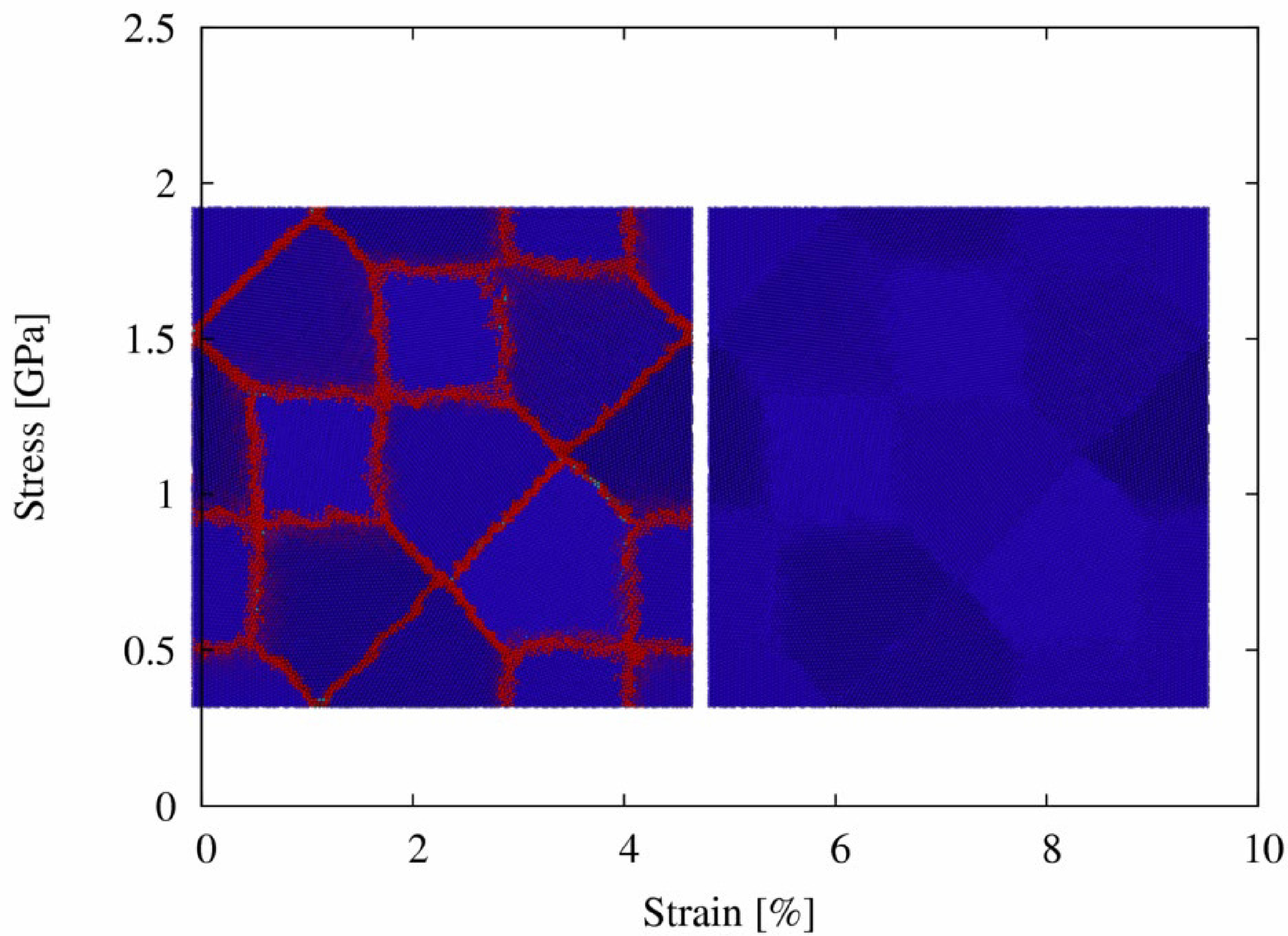
# Coupled Motion vs. Sliding: Pd



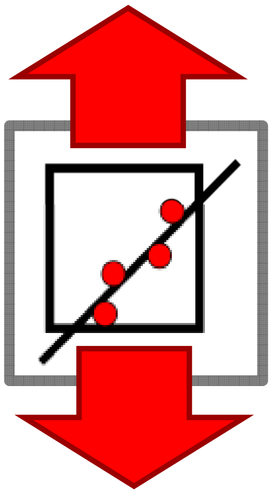


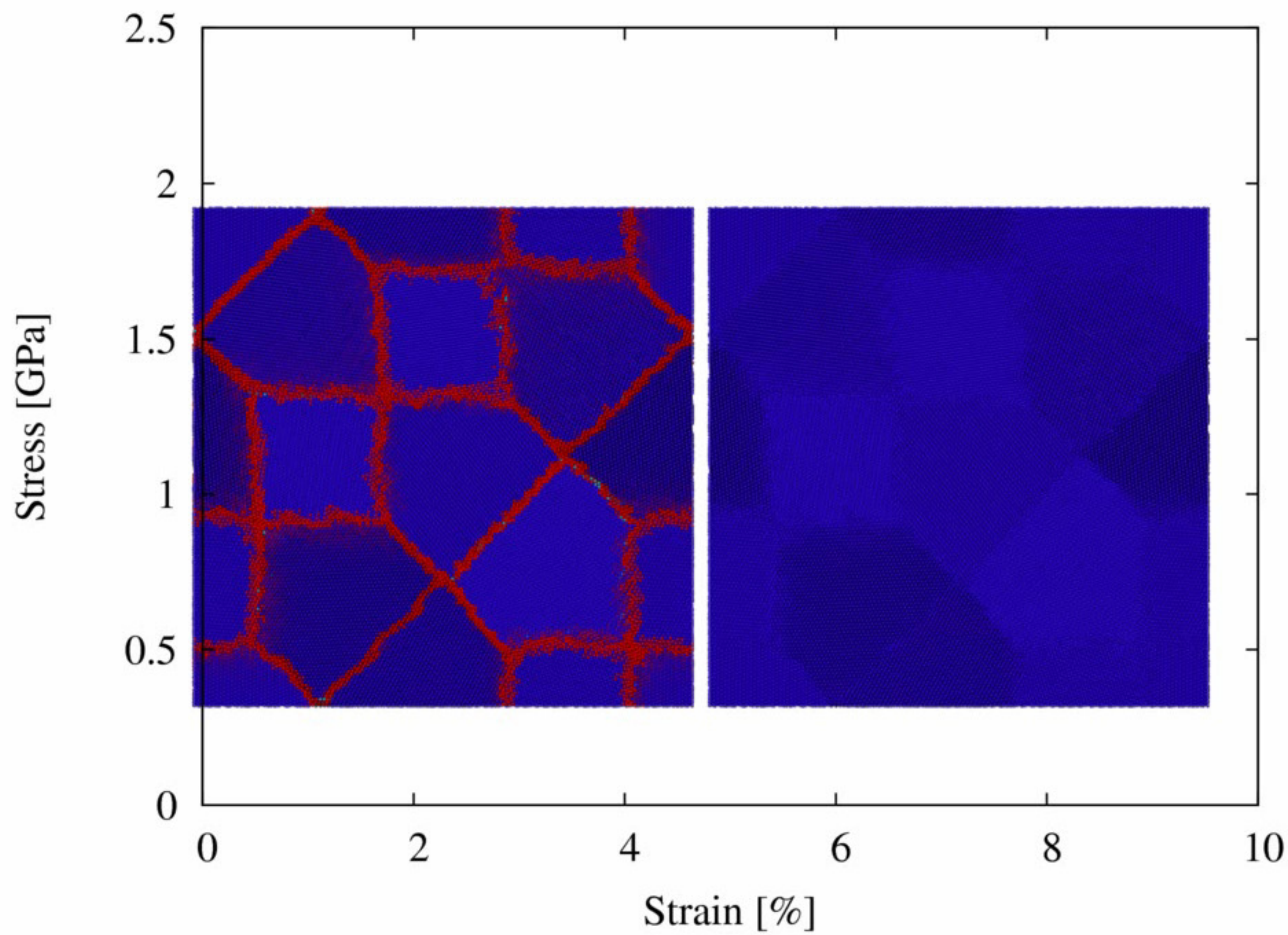
# Coupled Motion vs. Sliding: Pd



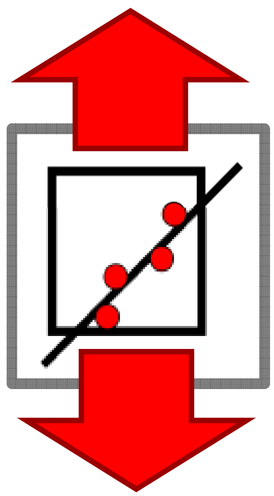


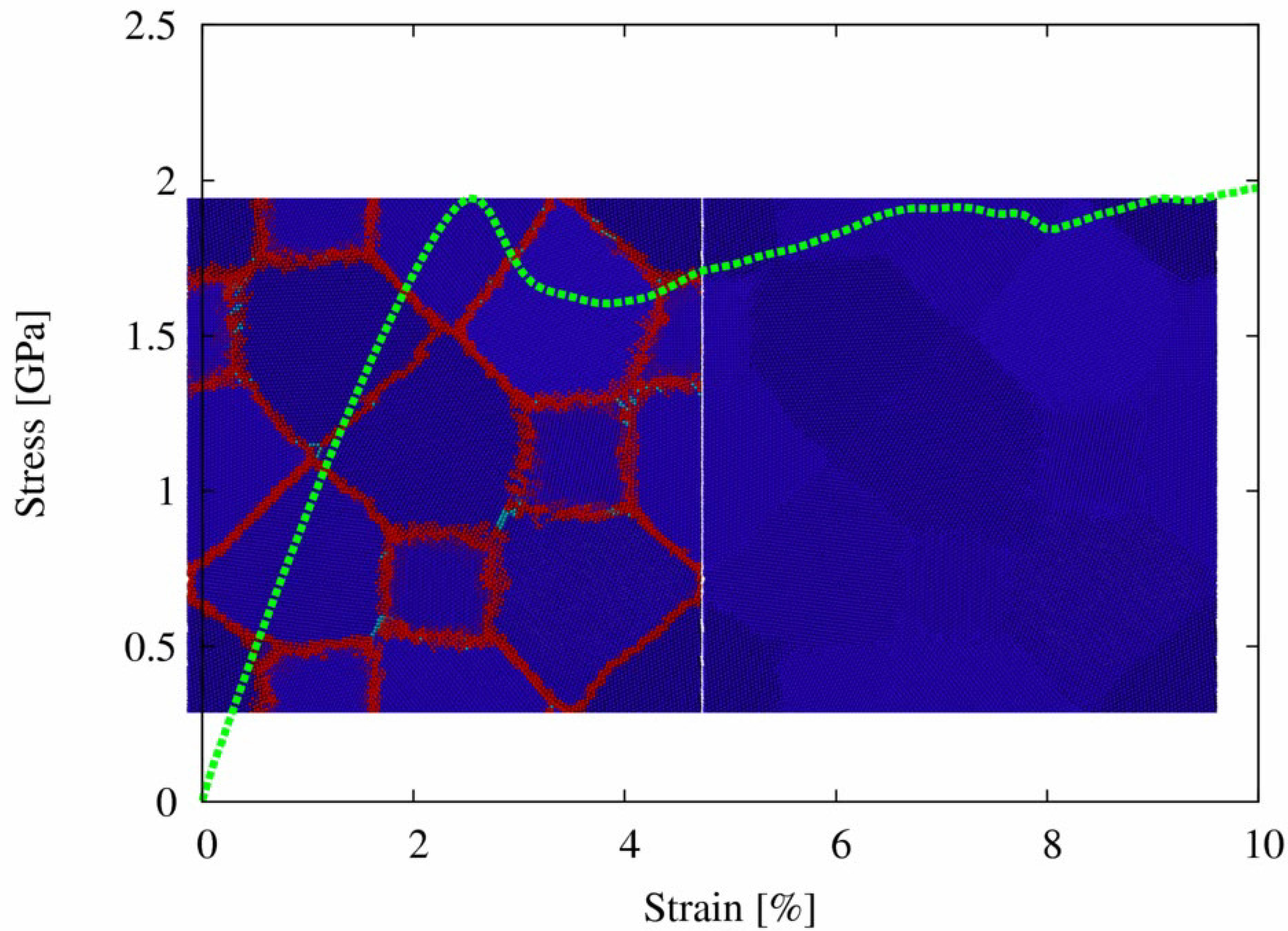
# Coupled Motion vs. Sliding: PdAu



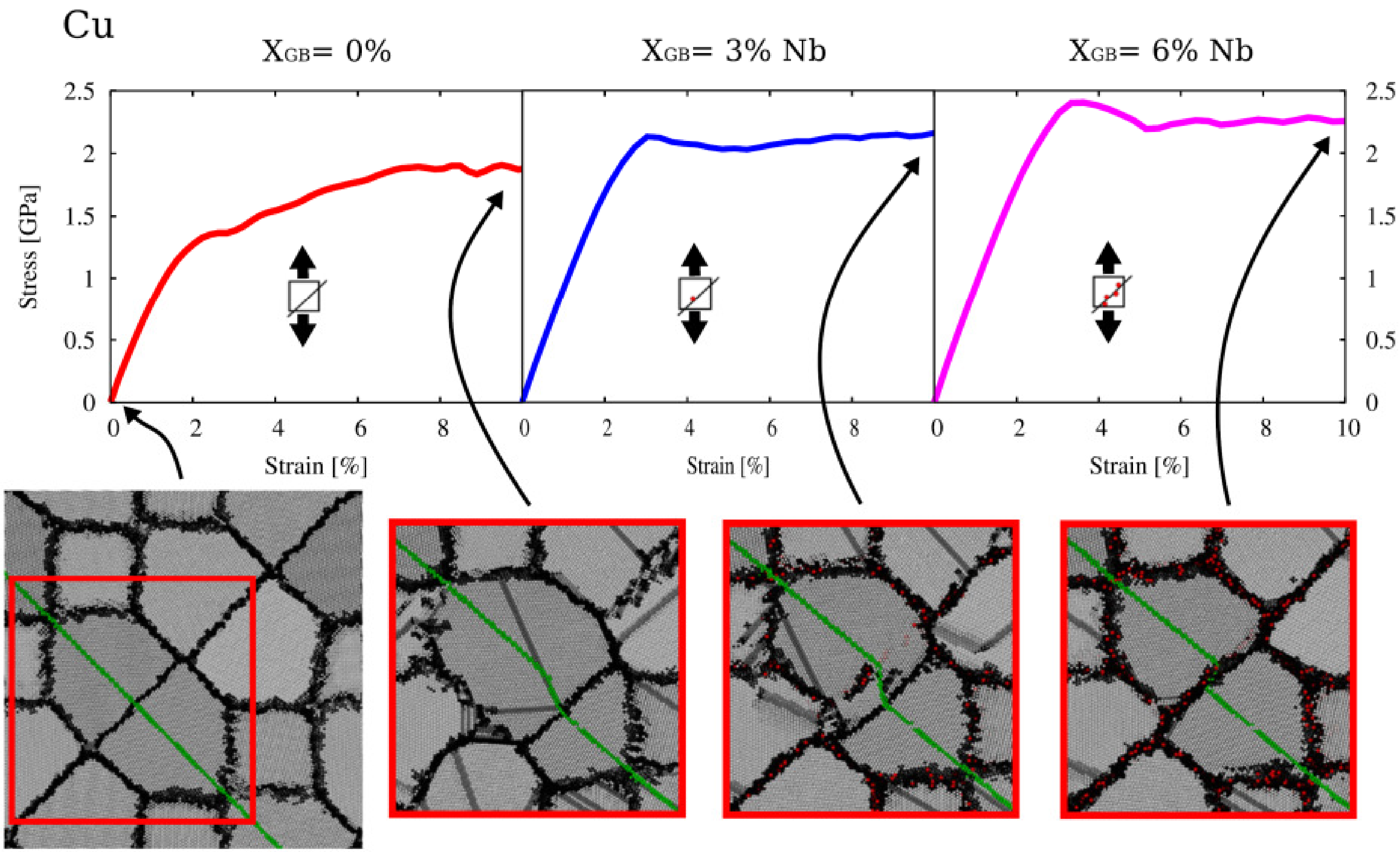


# Coupled Motion vs. Sliding: PdAu (with MC)





# Coupled Motion vs. Sliding: Cu-Nb



# Conclusions

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## The effect of miscible solutes

- The solute distribution in nc alloys is not necessarily homogeneous also for miscible solutes
- Miscible solutes increase the strength of the material for all studied grain sizes by decreasing the free volume in the GBs
- The GB composition is adjusting during deformation

## The role of the local kinetics

- Diffusional processes can alter the effect of miscible solutes
- If local kinetics allow for a sufficiently fast redistribution of solutes, no strengthening is observed
- The effect on the deformation mechanism was demonstrated for coupled GB motion

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