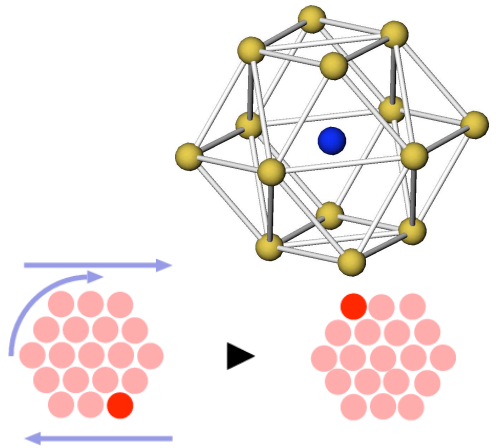
# Simulations of structural changes in metals during dry solid friction



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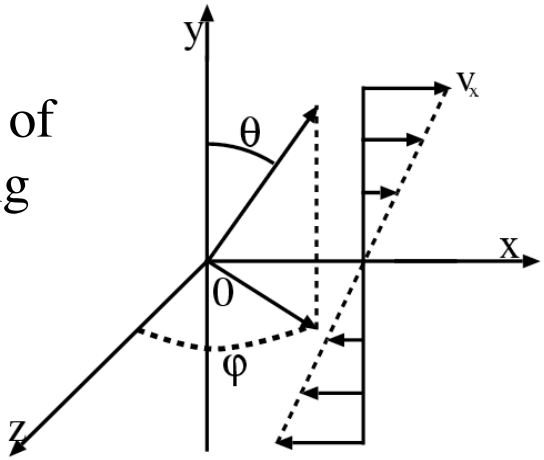
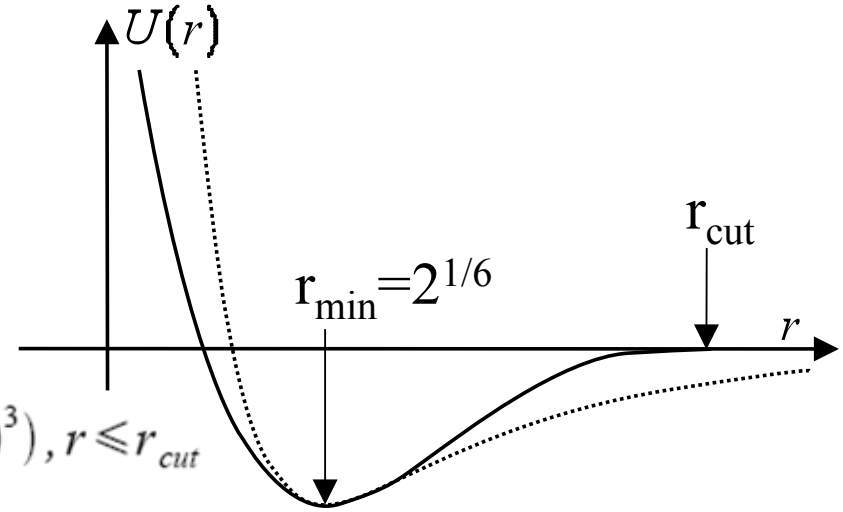
- low degree polynomial embedded-atom model metal
- influence of parameters on constitutive properties; embedded atom sponges and foams
- common neighbor structure analysis
- dry friction at metal-metal interfaces: transformation of structure, stationary structure and mechanical alloying
- conclusion and outlook



# Embedded atom model metal

$$E_{tot}=\sum_i\left(\sum_j \Phi(r_{ij})+F(\rho_i)\right)$$



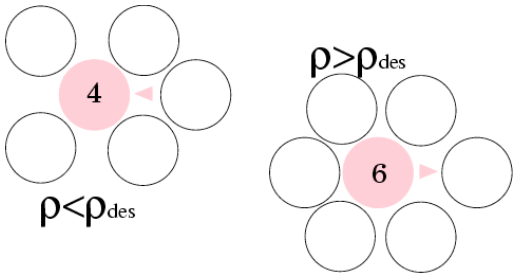

binary part

$$\Phi(r)=\phi_0 r_0^{-6}\left(3(r-r_{cut})^4-4(r_{cut}-r_{min})(r_{cut}-r)^3\right),\ r\leqslant r_{cut}$$

$$\Phi(r)=0,\ r>r_{cut}$$

embedding functional

$$F(\rho_i)=\phi_0\sum_{k=2,4,\ldots} r_0^3 k F_k\left((\rho_i-\rho_{des})^k-(w(0)-\rho_{des})^k\right)$$

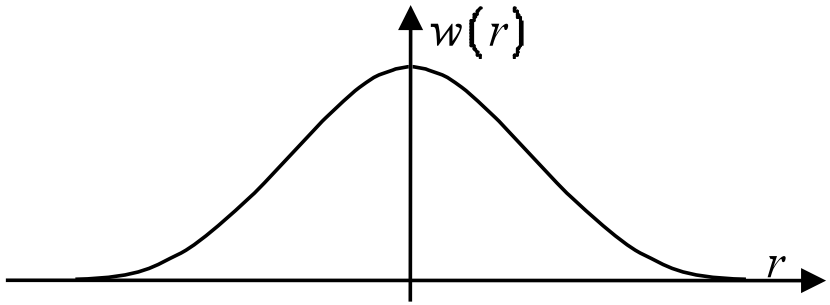



embedding density

$$\rho_i=\sum_j w(r_{ij})$$

Lucy's weight function

$$w(r)=w_0\left(1+3\frac{r}{r_{cut}}\right)\left(1-\frac{r}{r_{cut}}\right)^3$$



two-body interaction potential

$$\Phi(r)=\phi_0 r_0^{-6}(3(r-r_{cut})^4-4(r_{cut}-r_{min})(r_{cut}-r)^3)$$

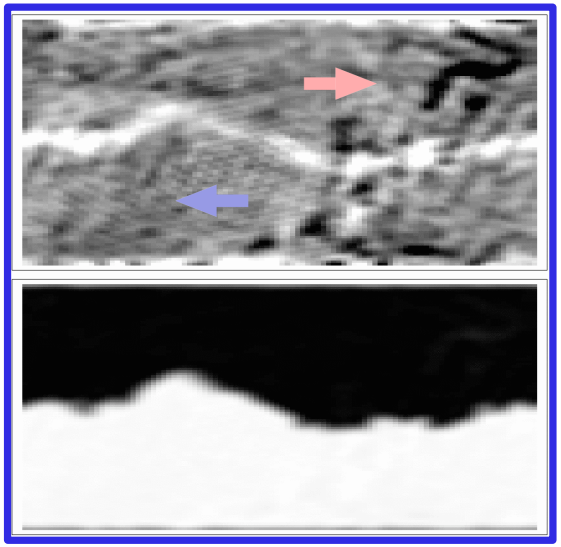
$$F(\rho_i)=\phi_0 \sum_{k=2,4,\ldots} r_0^3 k F_k((\rho_i-\rho_{des})^k-(w(0)-\rho_{des})^k)$$

embedding functional

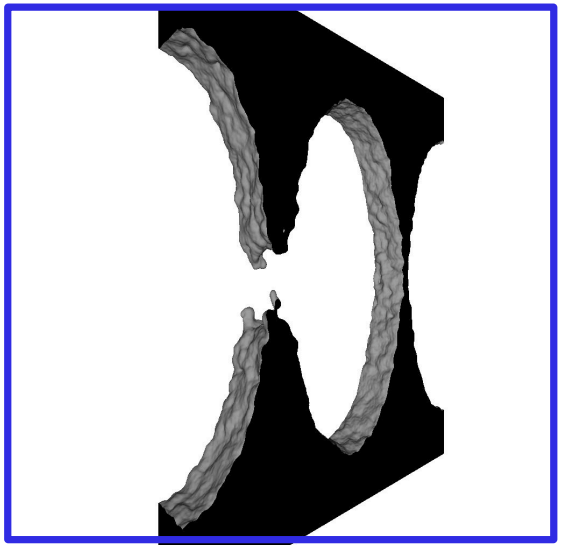
$\frac{E_{vac}}{E_{coh}}$, $\frac{C_{elast}}{E_{coh}}$ (bulk modulus B, $C_{11}$, $C_{12}$)

shear modulus G, $G_{44}$,

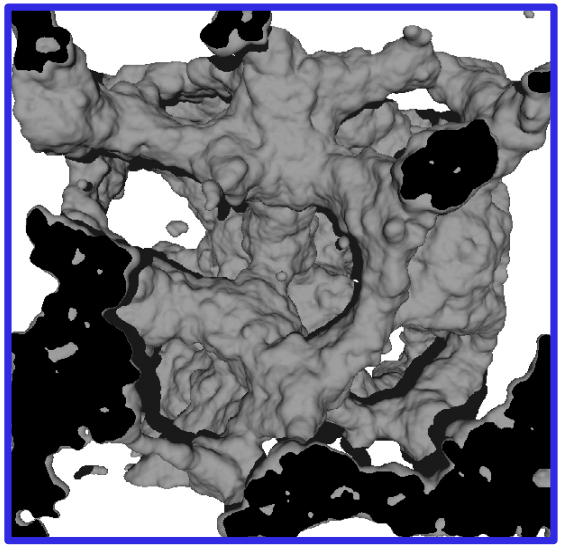
Cauchy pressure $(C_{11}-C_{12})/2$



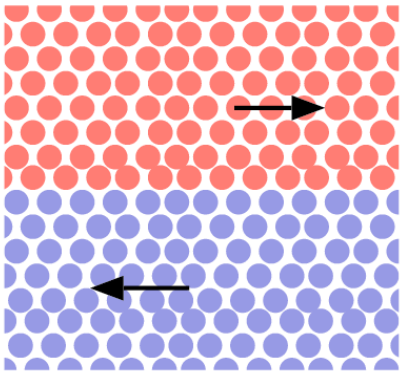
metal interface under steady shear flow

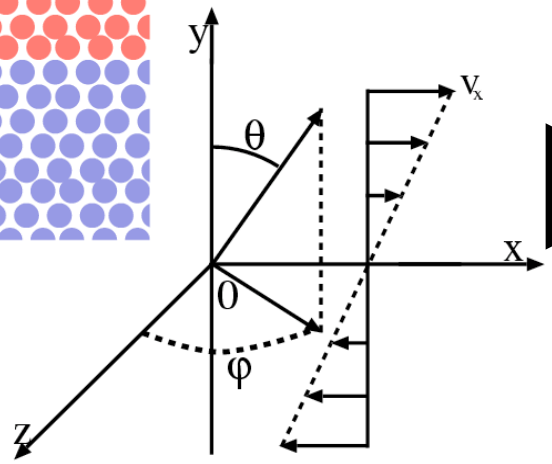


metallic foam walls

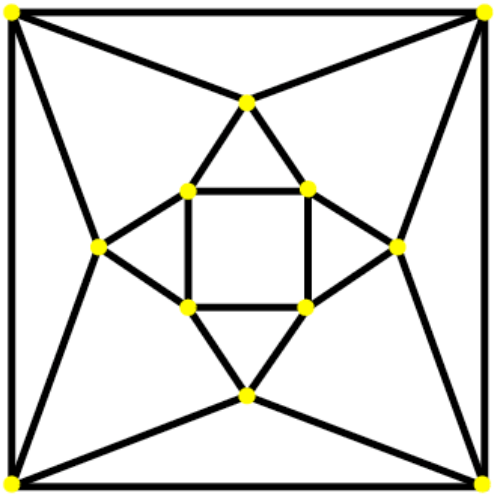


metallic sponges



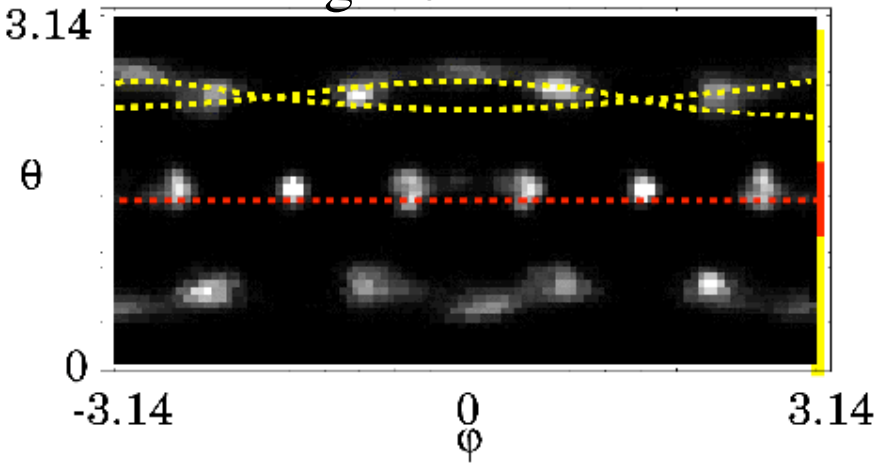


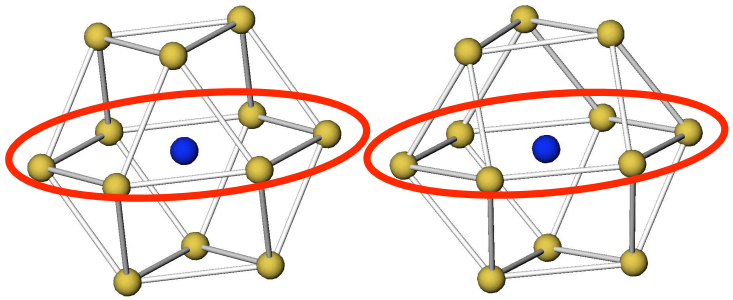

common neighbor analysis



planar graph

angular distribution of next neighbors



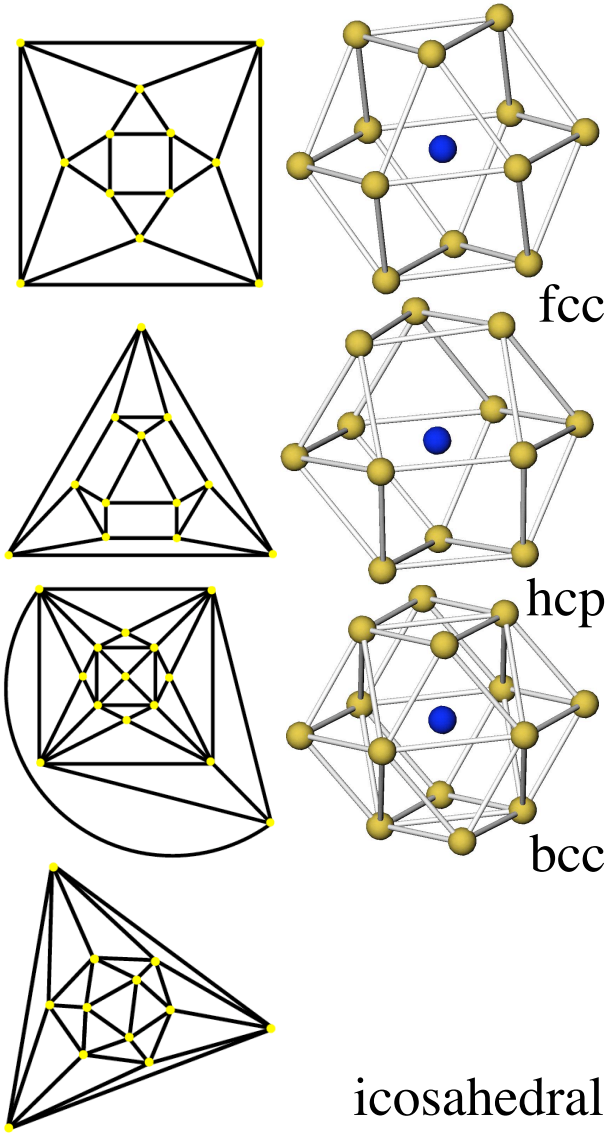



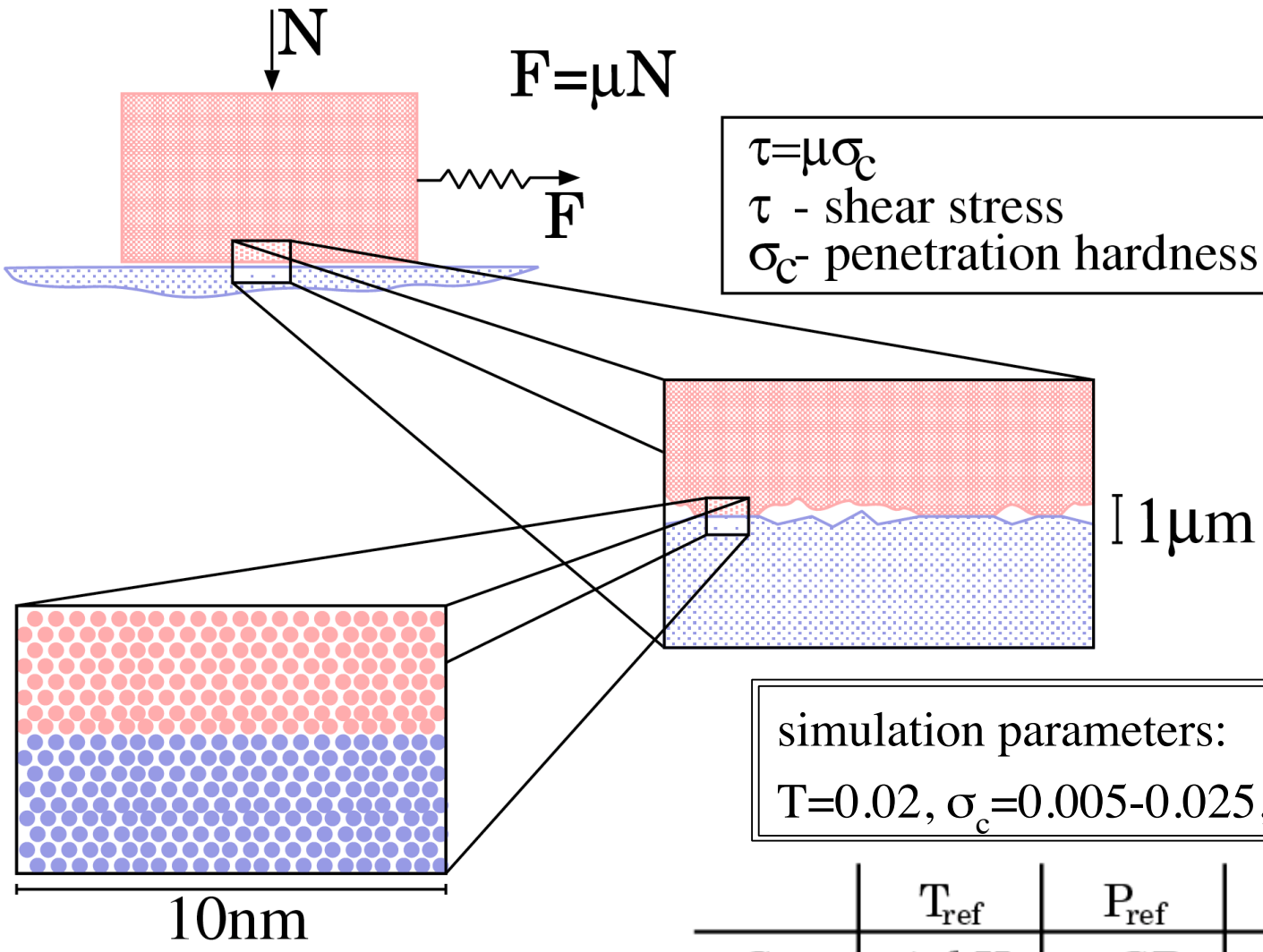
1. Planar graphs for each atom in simulation is created.

**2. <u>Topological</u> equivalence with planar graphs of ideal crystal structures is tested.**

3. Measure of the amount of certain crystal structure is ratio between

   all atoms within that structure (central atoms and their neighbours), and total number of atoms in the system.

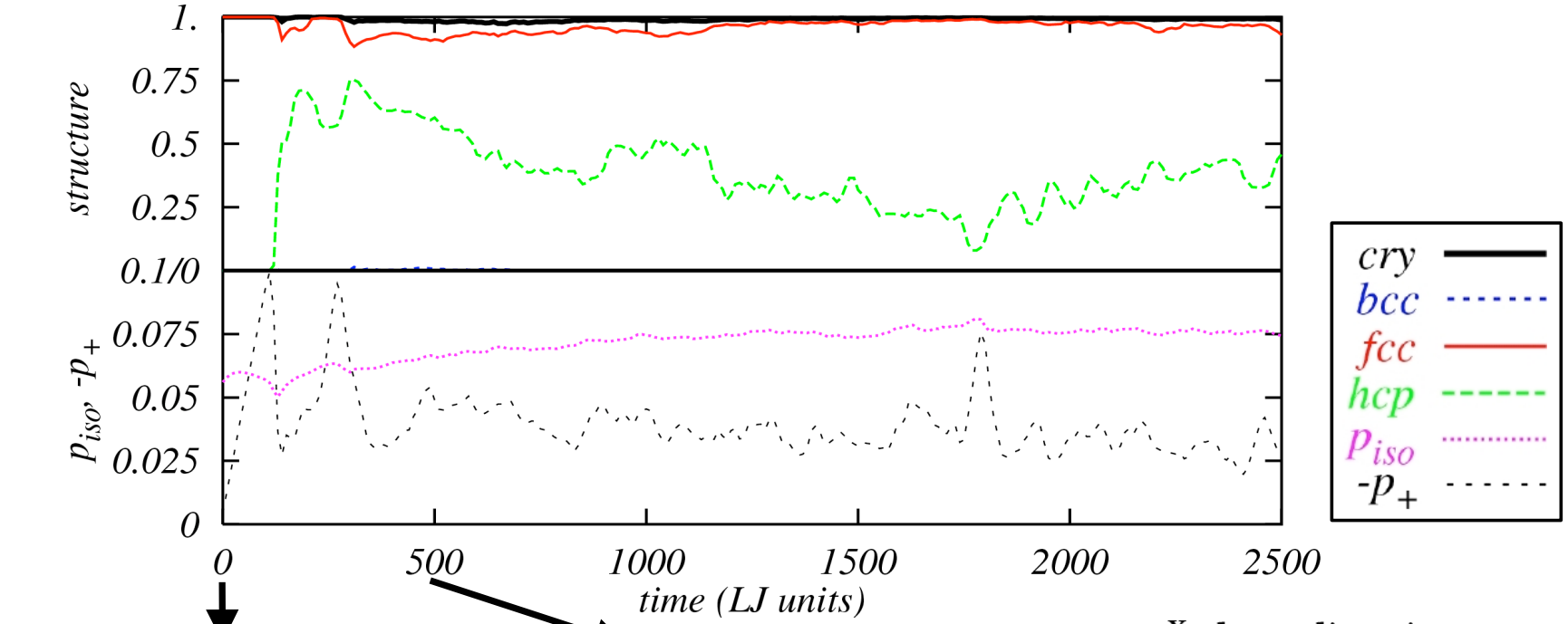


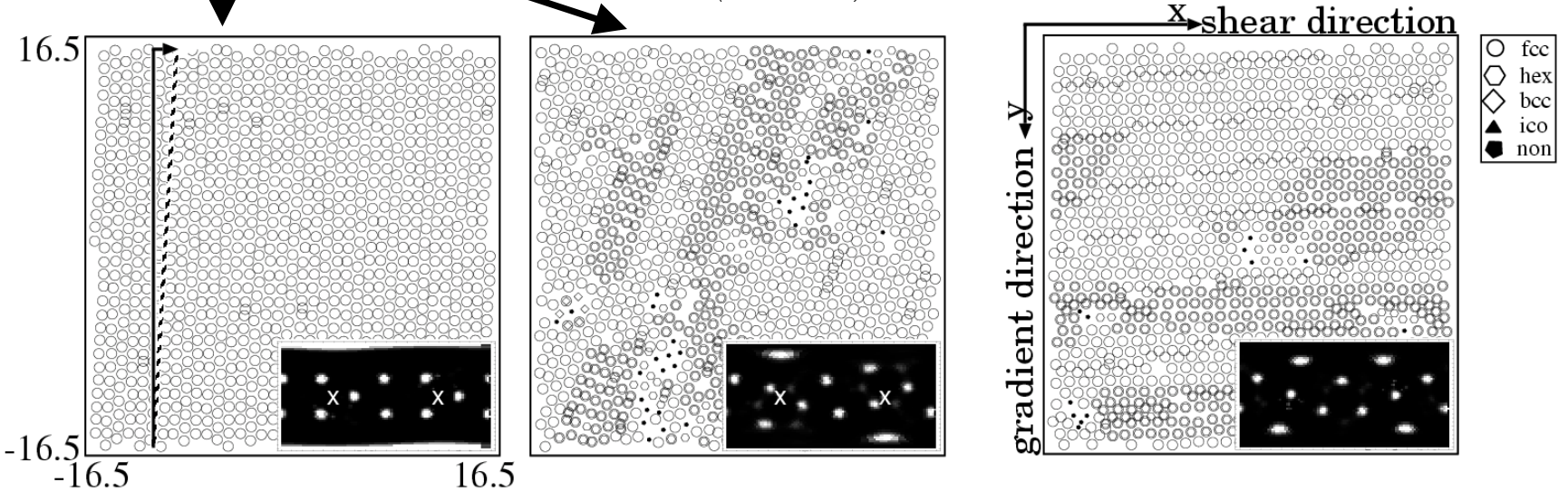



$\tau=\mu\sigma_c$
$\tau$ - shear stress
$\sigma_c$- penetration hardness

simulation parameters:
T=0.02, $\sigma_c$=0.005-0.025, n=1., $\gamma$=0.001

| | $T_{ref}$ | $P_{ref}$ | $r_{ref}$ | $t_{ref}$ |
|---|---|---|---|---|
| Cu | 42kK | 38GPa | 0.23nm | $0.97\text{x}10^{-13}$ |
| GEAM | 40kK | 40GPa | 0.24nm | $0.9\text{-}2\text{x}10^{-13}$ |



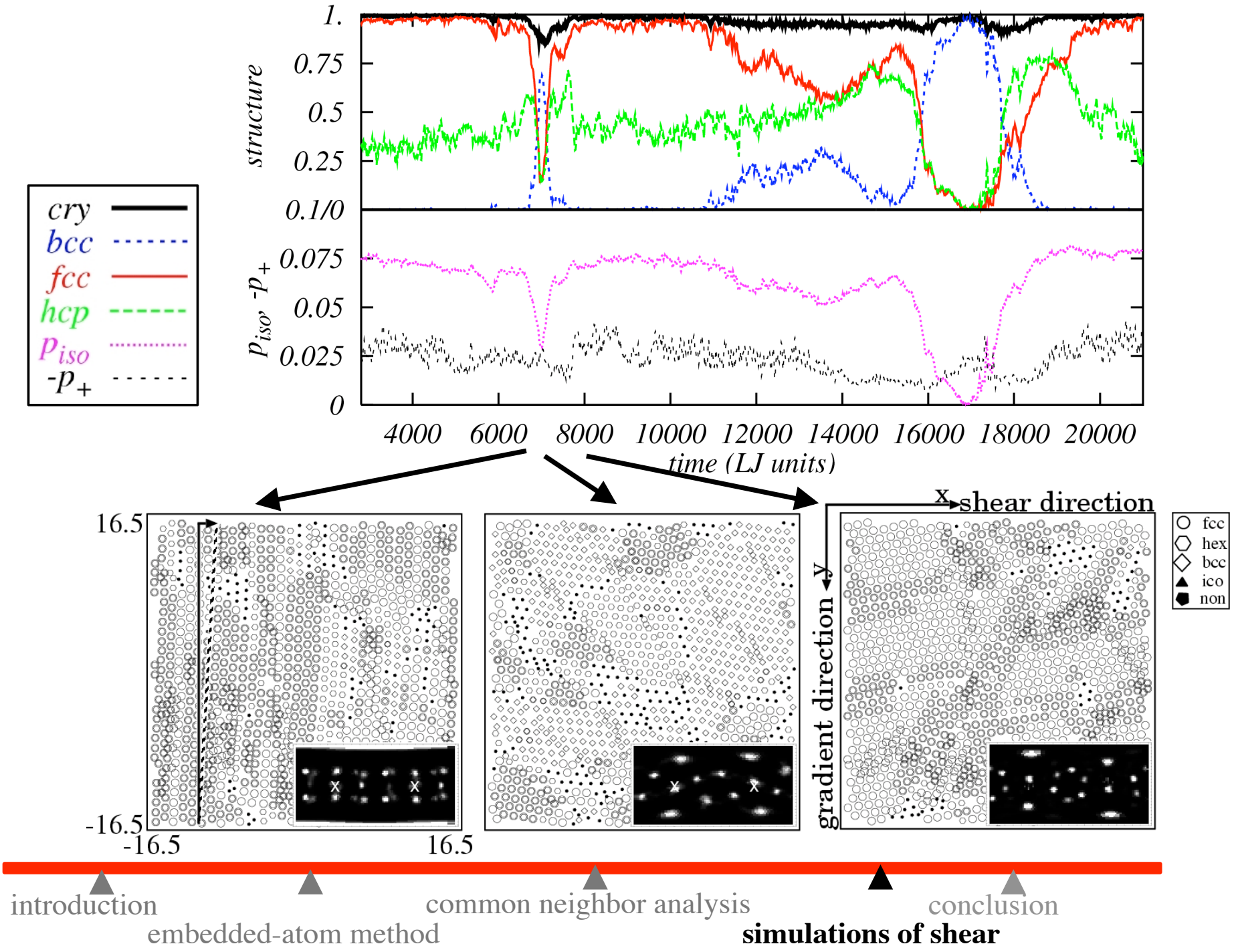

introduction

embedded-atom method

common neighbor analysis

**simulations of shear**

conclusion


cry
bcc
fcc
hcp
$p_{iso}$
$-p_+$
structure
1.
0.75
0.5
0.25
0.1/0
$p_{iso}$, $-p_+$
0.075
0.05
0.025
0
4000
6000
8000
10000
12000
14000
16000
18000
20000
time (LJ units)
16.5
-16.5
-16.5
16.5
x
shear direction
y
gradient direction
fcc
hex
bcc
ico
non
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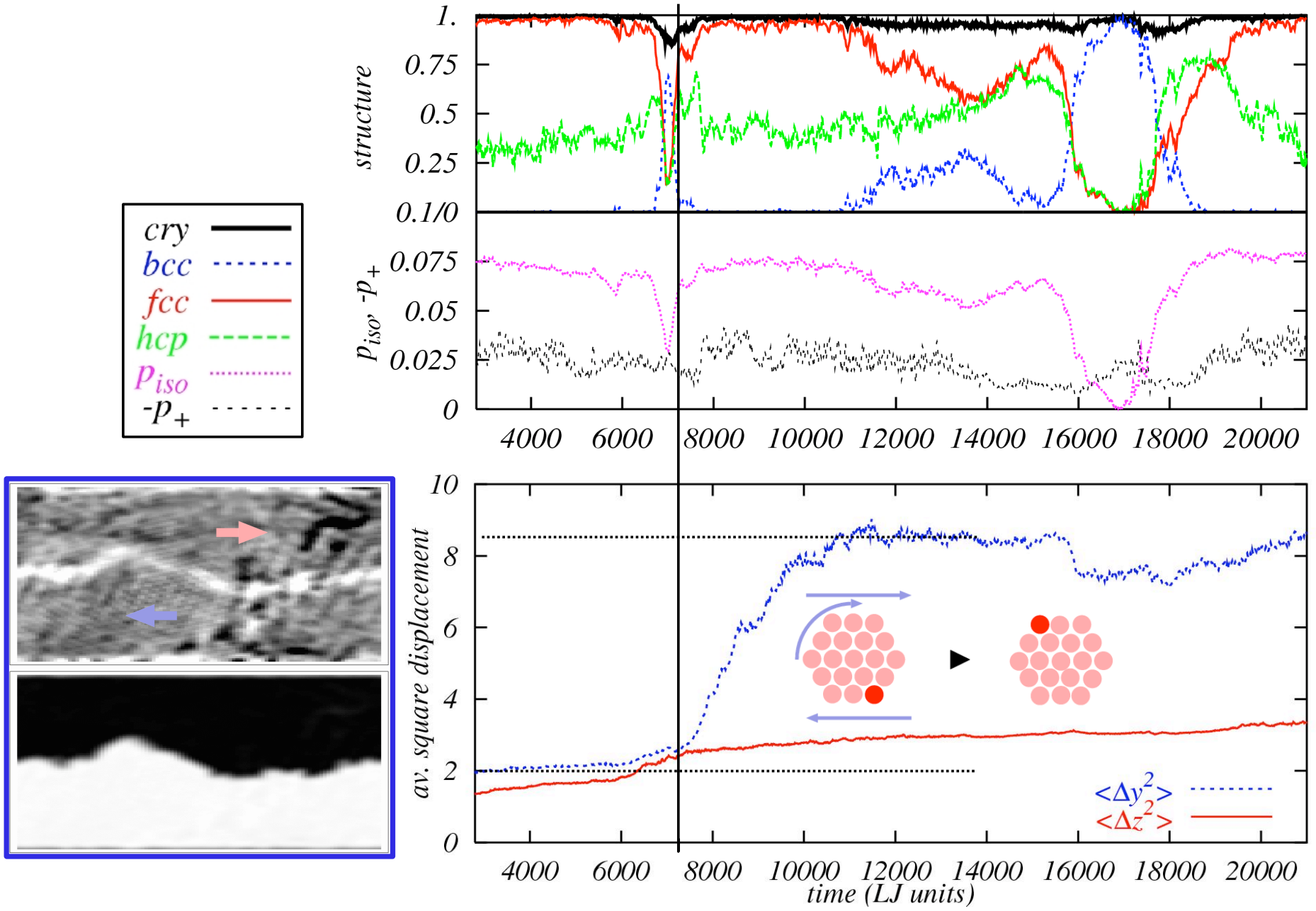


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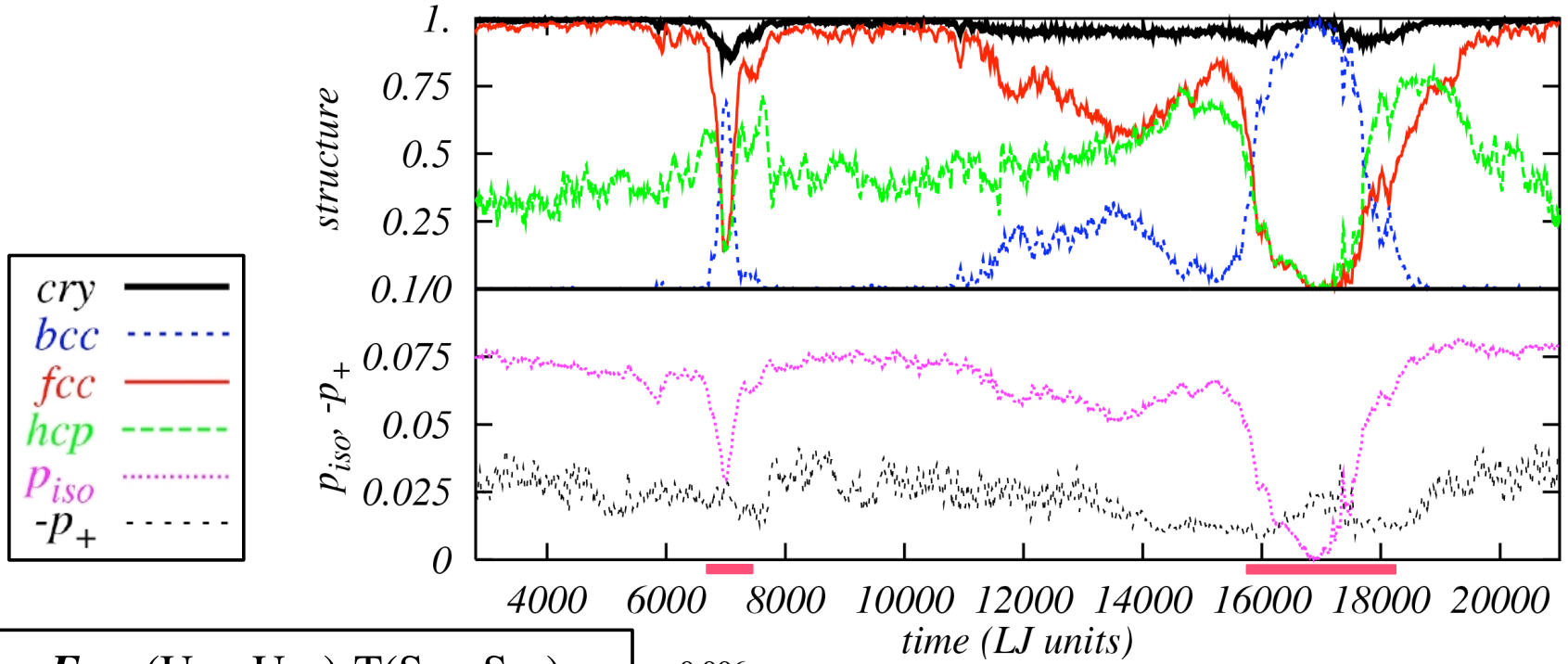
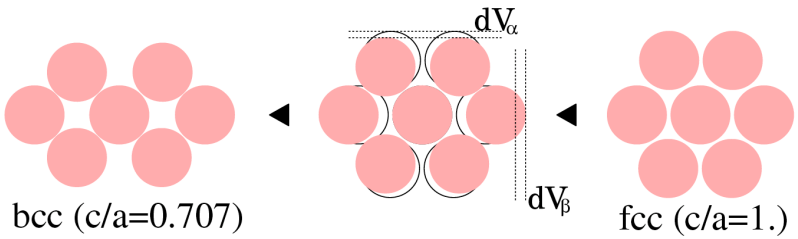
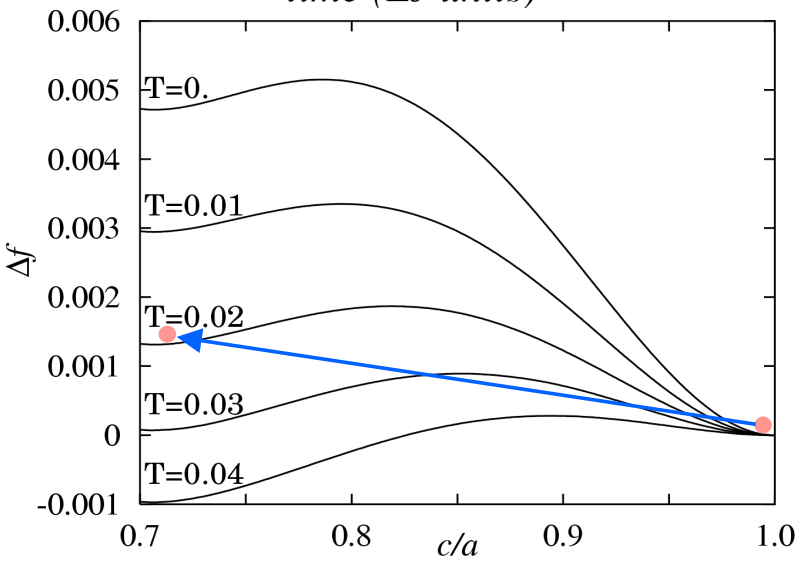


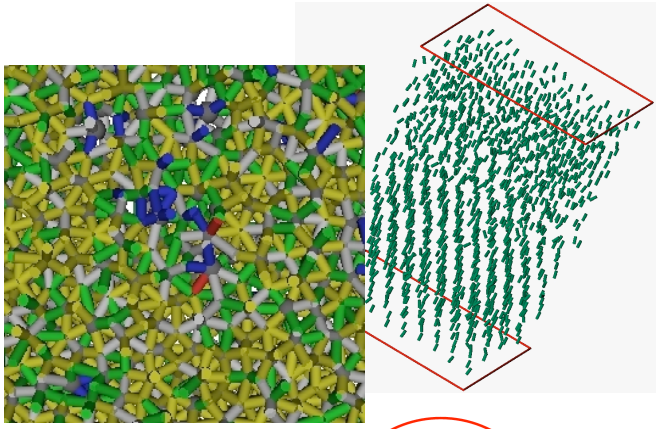

$$F_{bcc}-F_{fcc}=(U_{bcc}-U_{fcc})-T(S_{bcc}-S_{fcc})$$

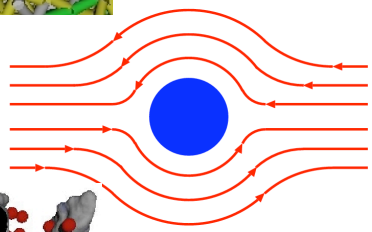
$f=-PdV-sdT$ $\quad T\equiv const$

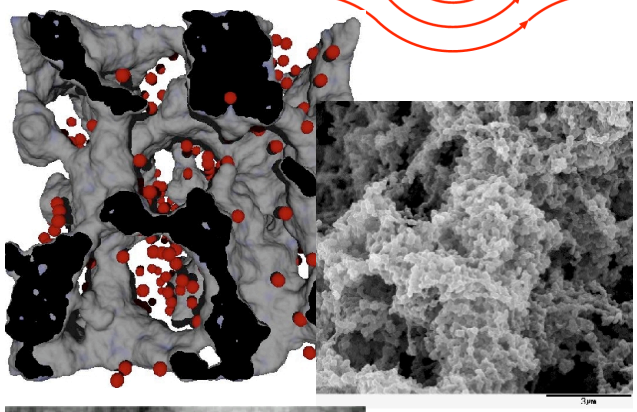
$df=-P_{\alpha\alpha}dV_{\alpha}$

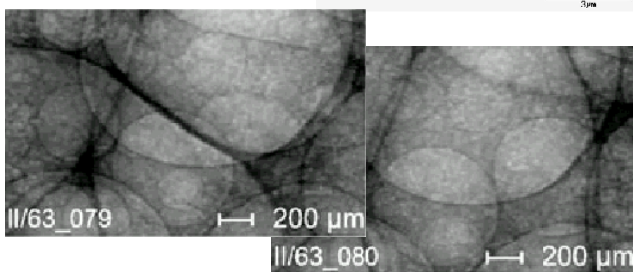






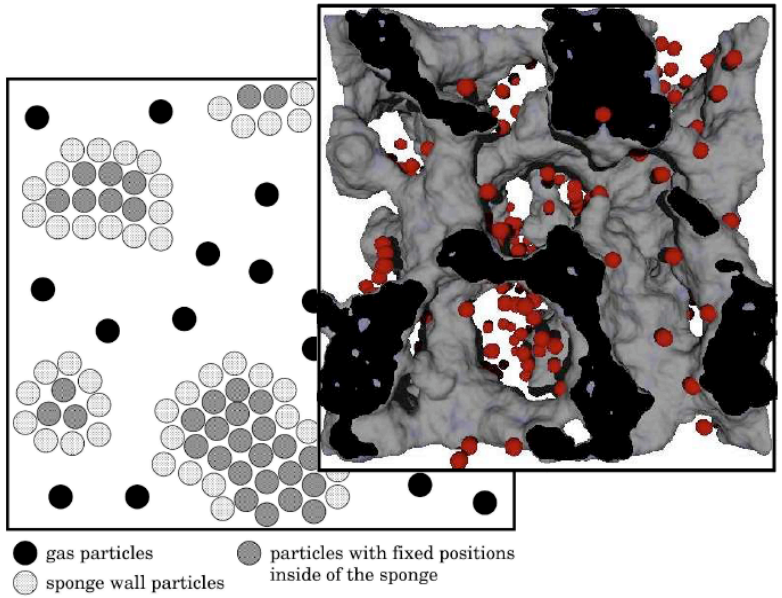





- ✓ low degree polynomial embedded atom method
- ✓ common neighbor analysis
- ✓ influence of modes of collective motion
- ✓ martensitic transformations (bcc>fcc>bcc)

Potential topics for further research:

- ✓ mechanical alloying at inhomogeneous $metal_1$-$metal_2$ interfaces
- ✓ to incorporate current simulation results in mesoscale methods; flow around inclusion
- ✓ diffusion and flow through embedded atom model sponges (+ chemical reactions & particle agglomeration)




**"Normal" diffusion: $\langle \Delta r^2 \rangle \sim t$**

Anomalous diffusion due to particle interaction $\langle \Delta r^2 \rangle \sim t^{\alpha}$, $\alpha < 1$

(chemical reaction, agglomeration)

- gas-gas interaction SHRAT (attractive)
- gas-wall interaction SHREP

$\Phi(r) = \phi r_0^{-4} (r - r_{min}^4)$, $r \le r_{min}$

$\Phi(r) = 0$, $r > r_{min}$

(repulsive)