Towards multiscale material modeling via computer simulations

Igor Stanković

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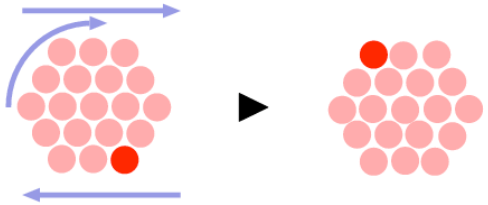
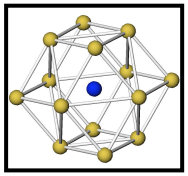
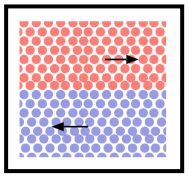


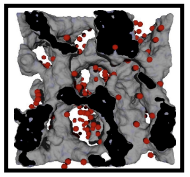
OUTLINE



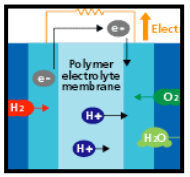
multiscale material modelling;
generic model for metals



simulations of dry friction in metals



simulations of the flow in porous media



outlook

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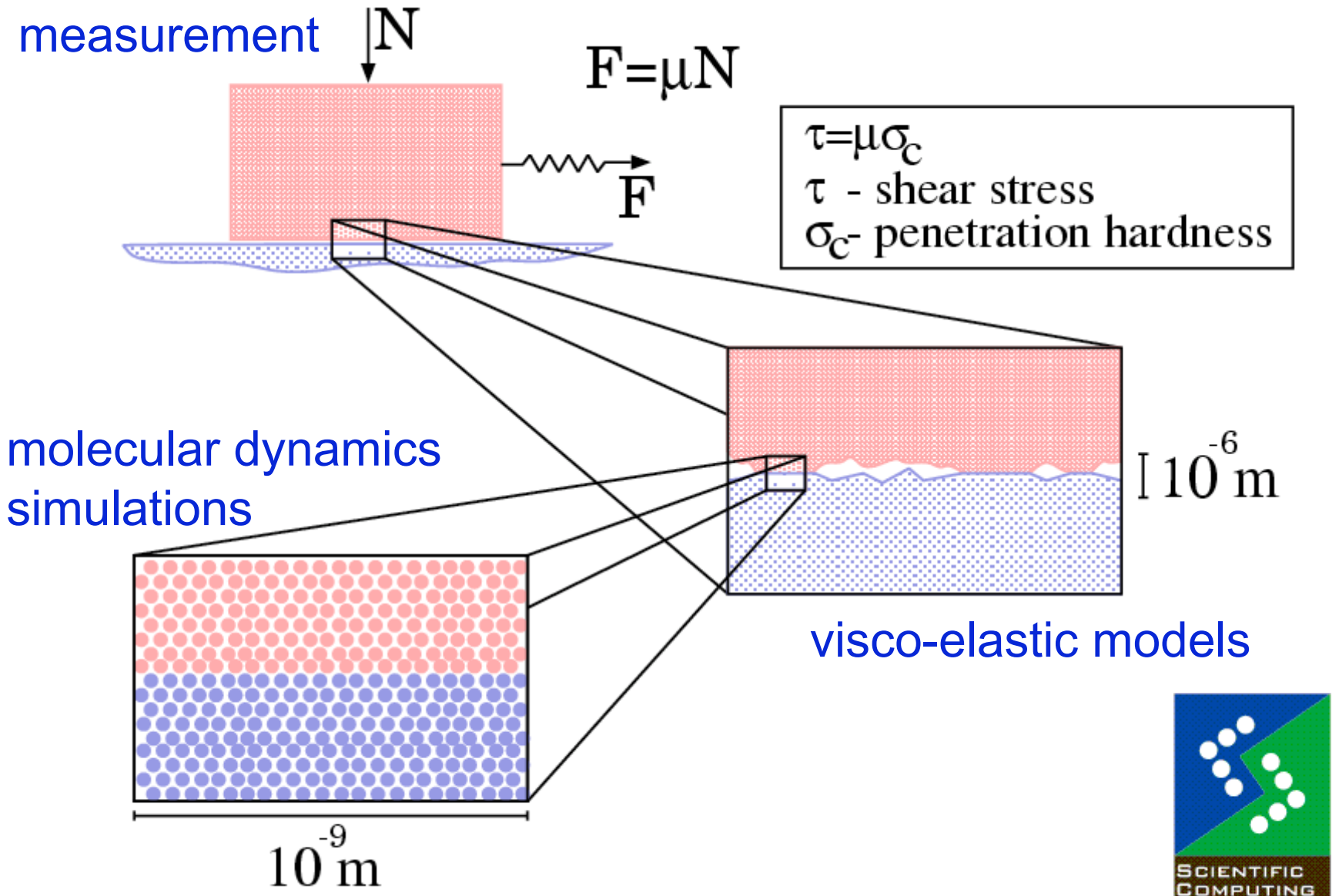
measurement
N
F=μN
F
τ=μσc
τ - shear stress
σc- penetration hardness
molecular dynamics
simulations
10-6 m
visco-elastic models
10-9 m
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Generic Embedded Atom Method (GEAM):

- ✓ *ab initio* motivated many-particle method
- ✓ generic - reproduces main properties of a number of real metals (Cu, Ni, Ag, Au, Pt, Pd)
- ✓ controlled by a set of basic model parameters
- ✓ computationally efficient

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$
$$\dot{\mathbf{v}}_i = -\nabla_i V(\mathbf{r}_1, .., \mathbf{r}_N)$$

molekuli, atomi

$$V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \sum_i \sum_{j>i} \phi(|\mathbf{r}_i - \mathbf{r}_j|)$$

$$\phi_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

metali, poluprovodnici

$$V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \sum_i \left(\sum_{j>i} \phi(|\mathbf{r}_i - \mathbf{r}_j|) + \Theta(\rho_i) \right)$$

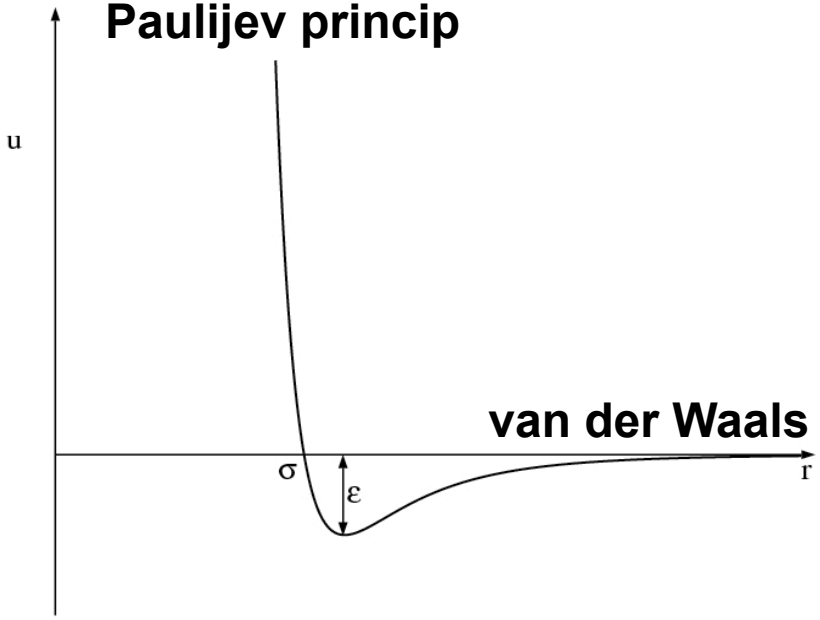
$$\Theta(\rho_i) = \phi_0 \sum_{k=2,4,...} r_0^3 k F_k ((\rho_i - \rho_{des})^k - (w(0) - \rho_{des})^k)$$

lokalna gustina

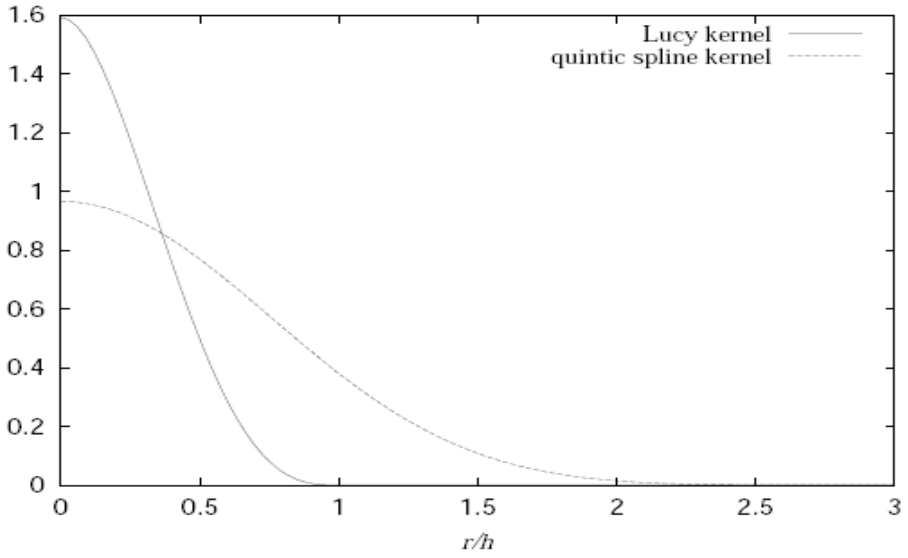
$$\rho_i = \sum_j w(r_{ij})$$

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

Paulijev princip



van der Waals



Metod molekularne dinamike

$$V(t)=\sum_i \sum_{j>i} \phi(|\mathbf{r}_i(t)-\mathbf{r}_j(t)|)$$ potencijalna energija

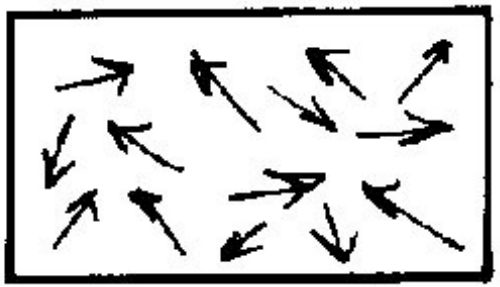
$$K(t)=\frac{1}{2}\sum_i m_i\left[v_i(t)\right]^2$$ kinetička energija

$$E(t)=K(t)+V(t)$$

$$K(t)=\frac{3}{2}N k_B T(t)$$ temperatura

$$PV = N k_B T-\frac{1}{3}\langle\sum_i \mathbf{r}_i\cdot\mathbf{F}_i\rangle$$ pritisak

$$D=\lim_{t\to\infty}\frac{1}{6t}\langle|\mathbf{r}(t)-\mathbf{r}(0)|^2\rangle$$ koeficijent difuzije



$\{q_i, p_i\}$

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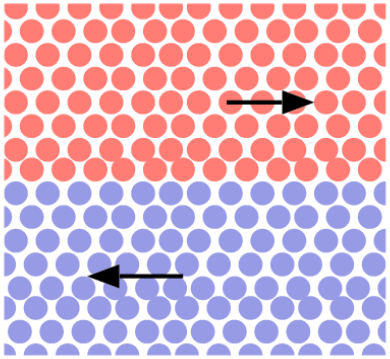
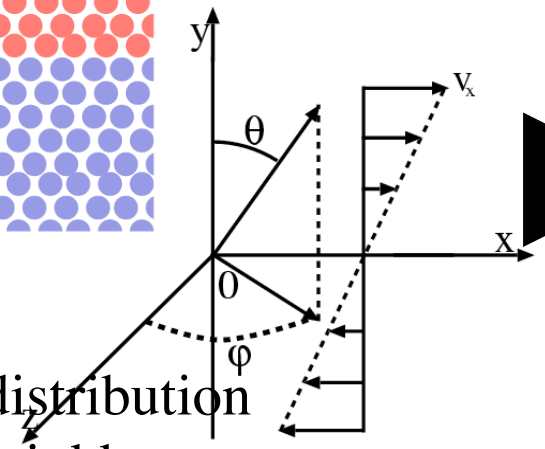
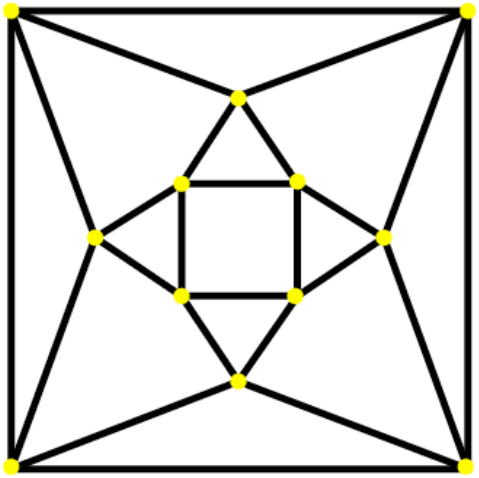
Common neighbour structure analysis



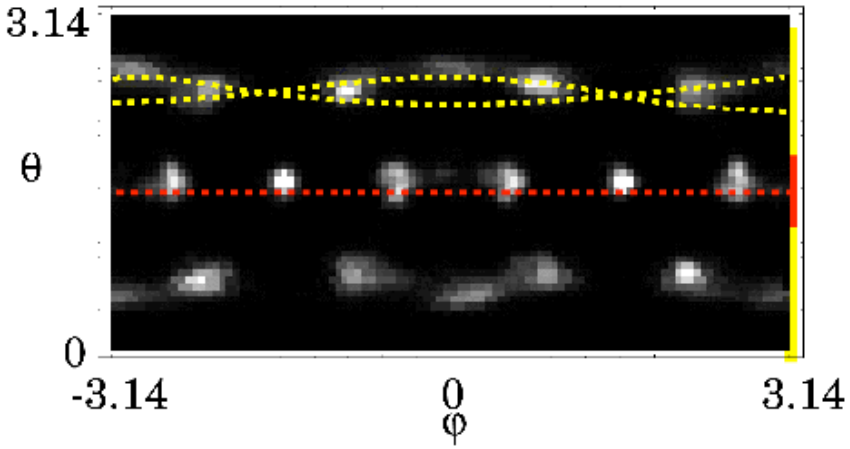


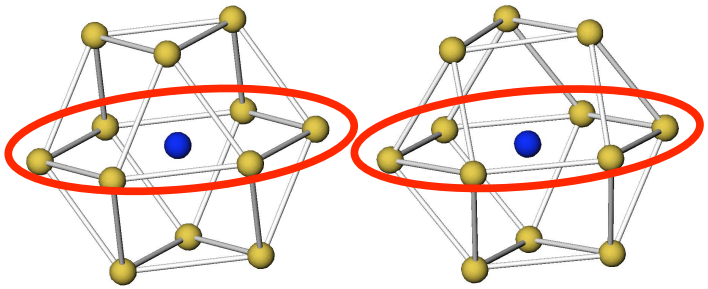
angular distribution
of next neighbors

common neighbor analysis

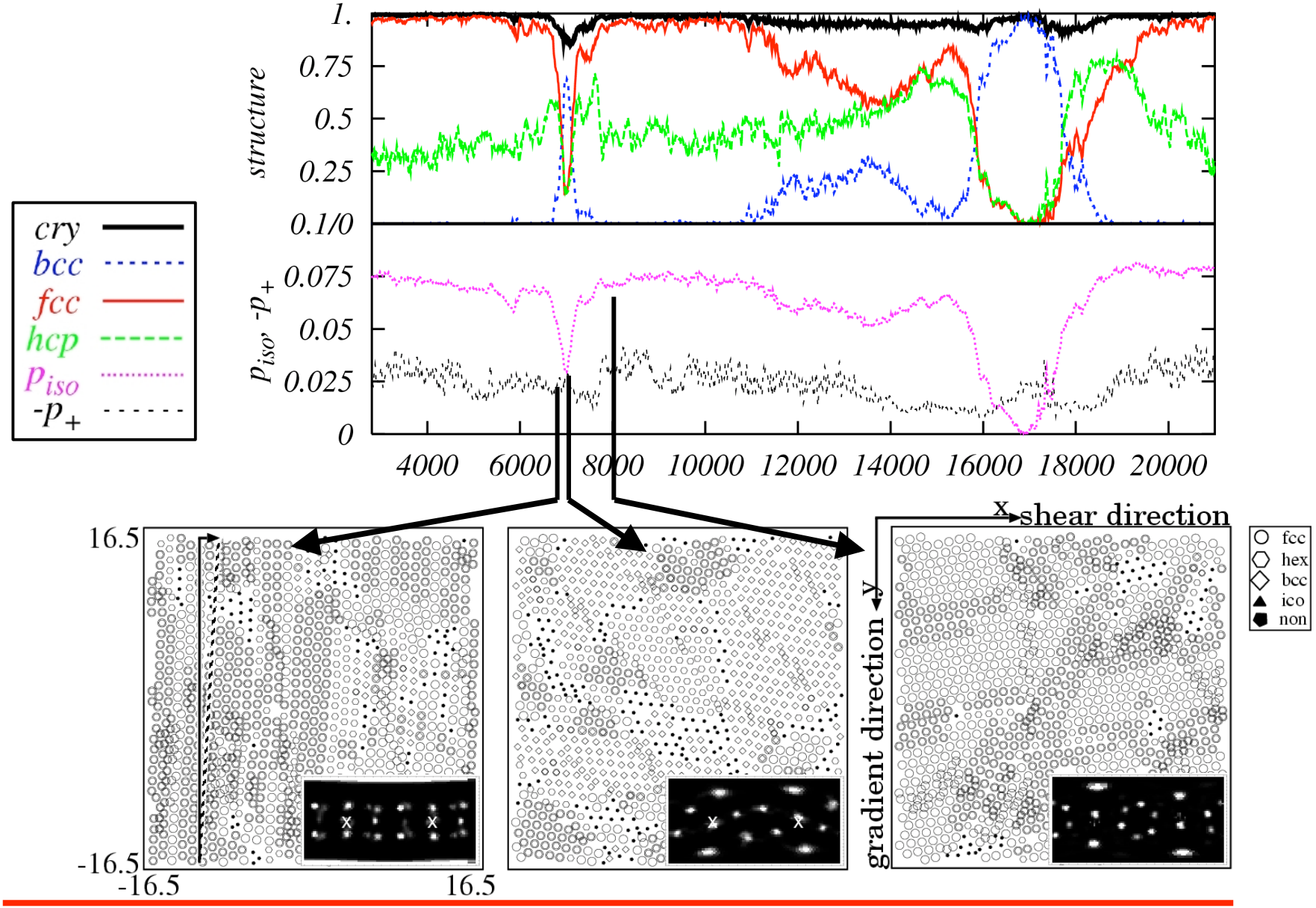


planar graph

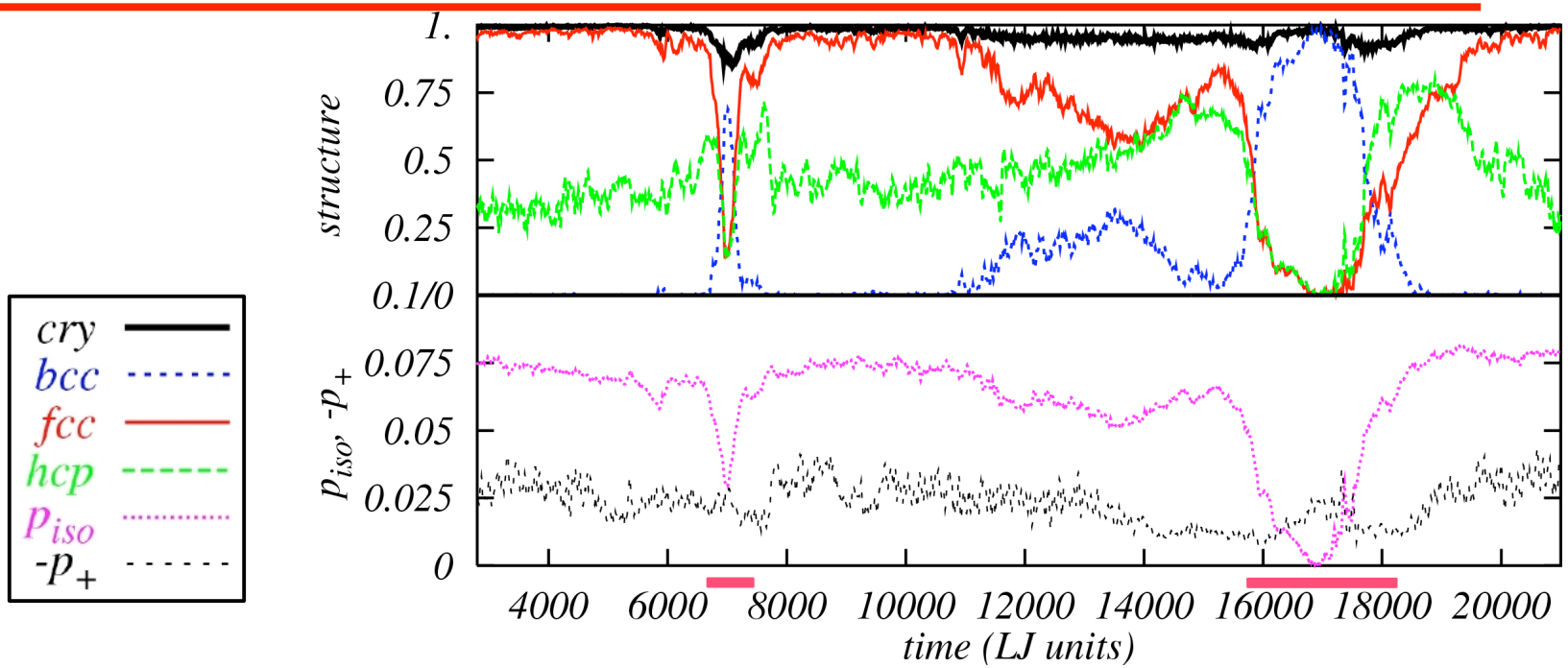




FCC-BCC-FCC transformation under shear



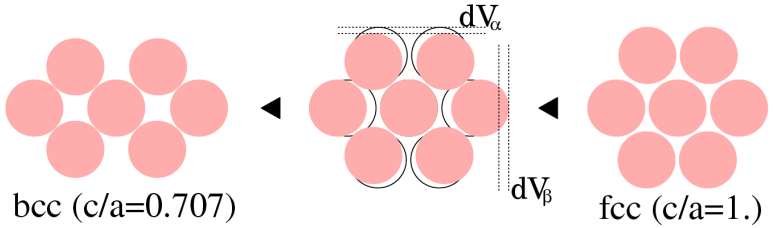
FCC-BCC-FCC transformation under shear

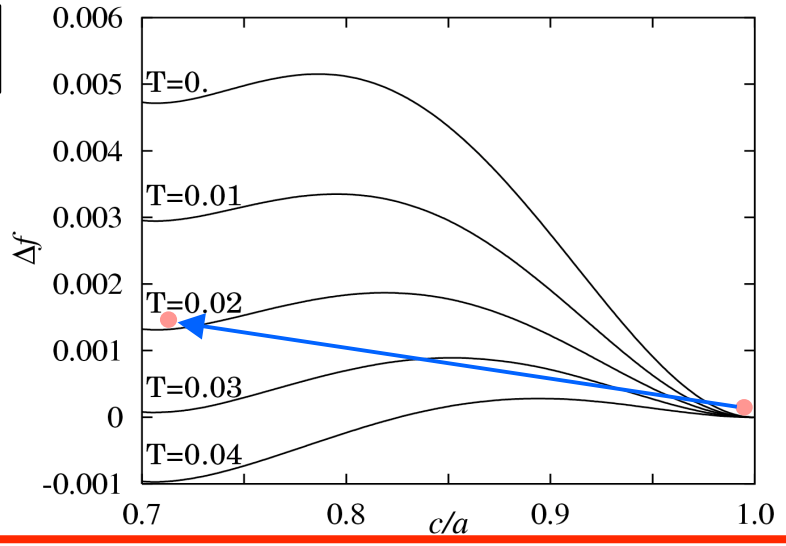


$$F_{bcc}-F_{fcc}=(U_{bcc}-U_{fcc})-T(S_{bcc}-S_{fcc})$$

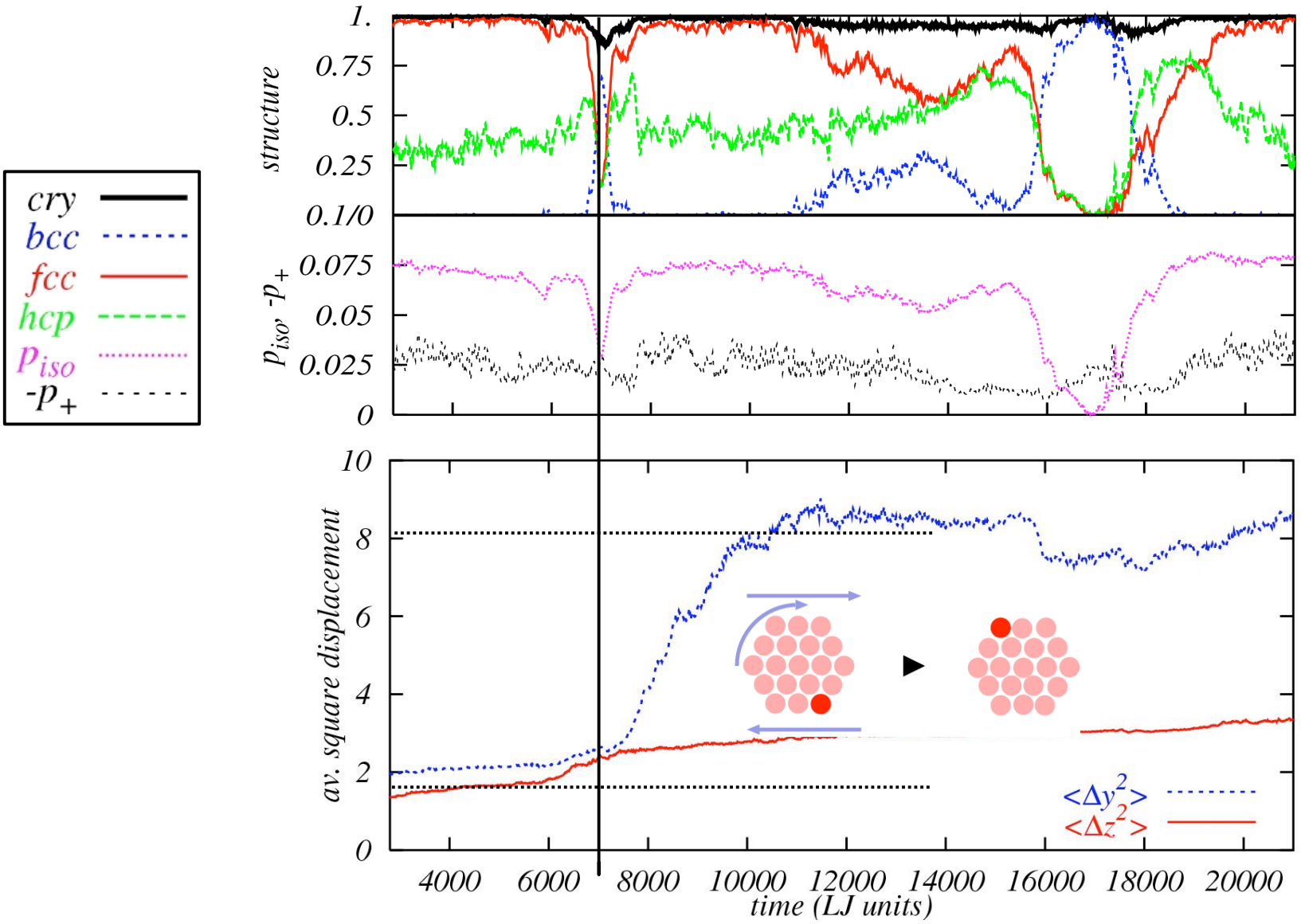
$f=-PdV-sdT$ $\quad T\equiv const$

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

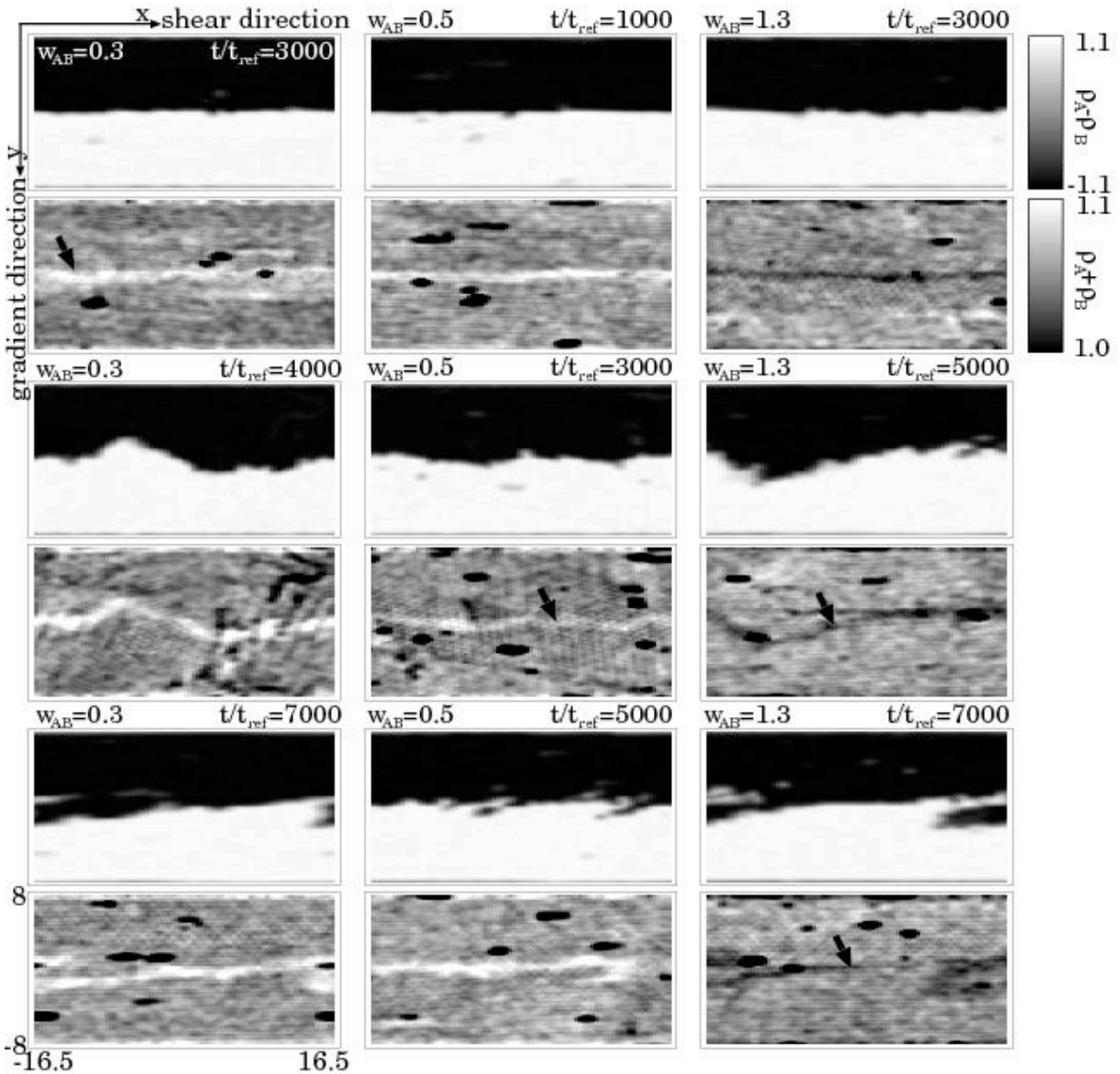


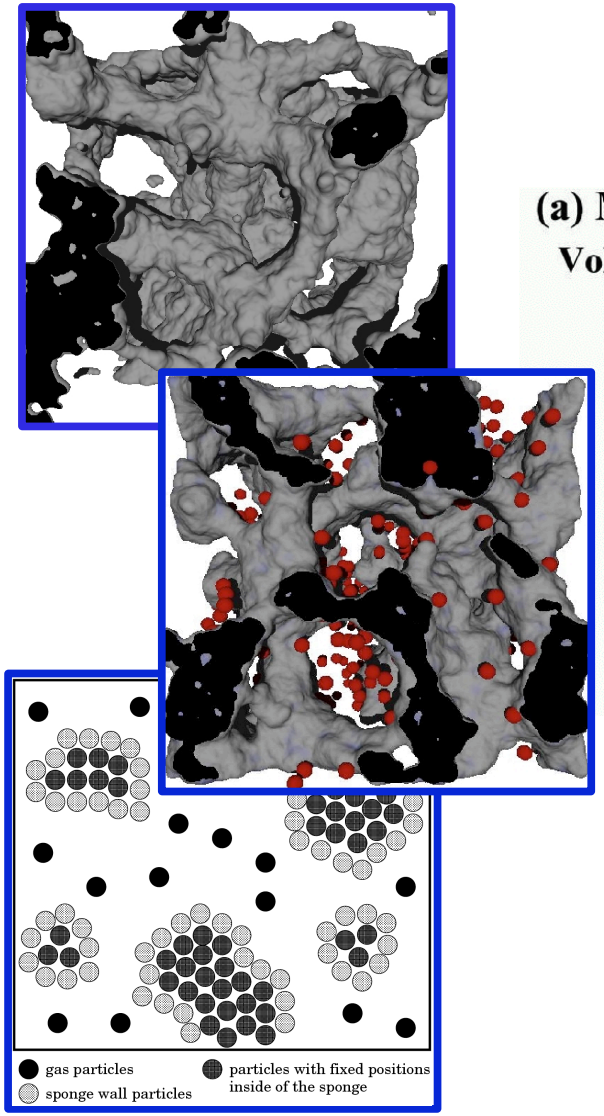


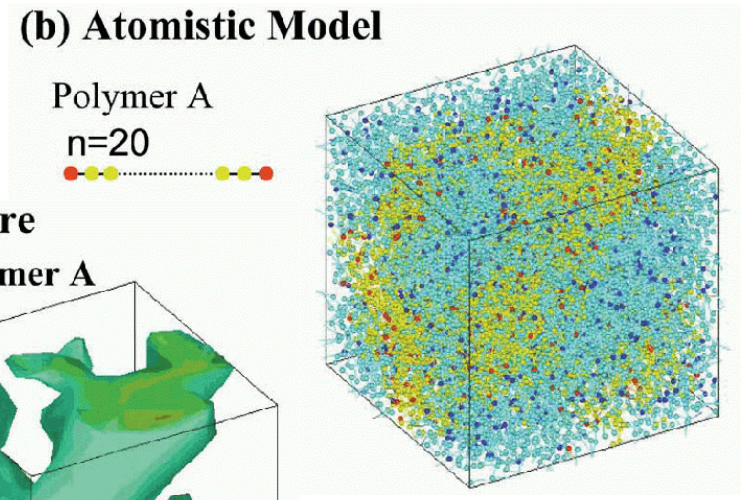
Mechanical mixing in sliding contact

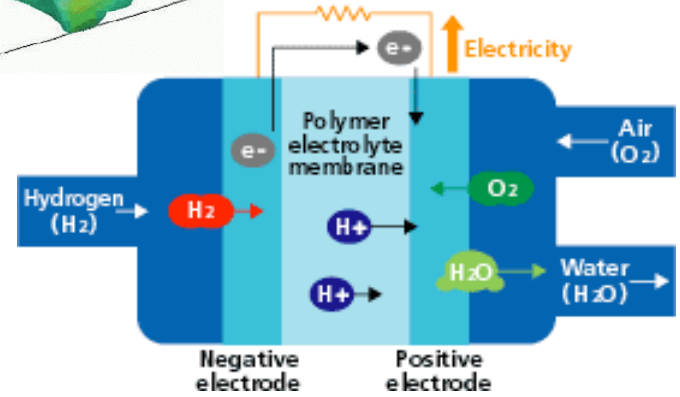


Mechanical mixing in sliding contact





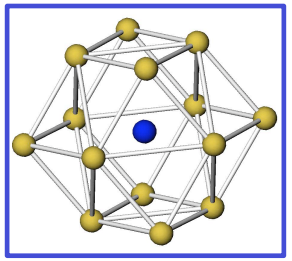




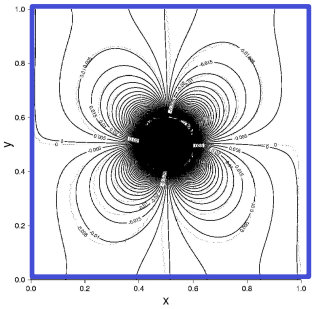
from nanoscale to macroscale:

... or maybe nano-particle aglomeration and deposition

flow in porous media

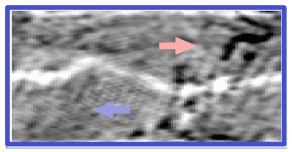


structural transformation due to the combined effect of temperature and pressure

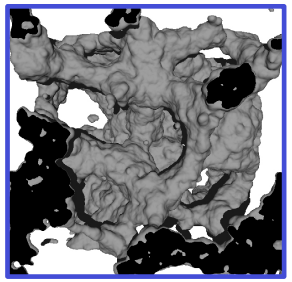


friction stress falls with temperature

mechanical alloying at sliding interface



embedded atom sponges and evolution of metallic foam walls



transport of reacting/agglomerating particles in porous media

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