Research Activities - Jörg Rottler

Development and application of computational methods for
the study of (soft) material behavior:

- in out-of-equilibrium situations
- from the nanoscale (often fluctuation-dominated) to the continuum (bulk behavior)

Focus areas:

1. How things break: mechanical behavior of amorphous materials such as metallic and polymer glasses, also soft glasses (colloids, etc.)
2. Modeling of charged (bio)molecular systems though novel algorithms
3. Microstructural evolution during thin film growth

Goals:

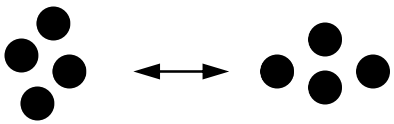
→ understand the molecular origins of macroscopic material properties

→ theory and modeling as a guide for the design of new materials

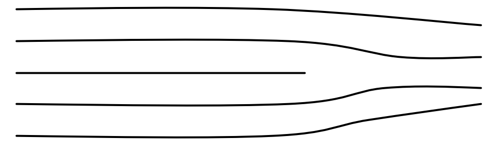
Deformation of disordered (glassy) matter

- Glassy materials exhibit slow dynamics and relaxation times longer than experimental timescales
- What is the elementary mechanism of deformation?

  Shear transformation zone (amorph)

  Dislocation (crystal)

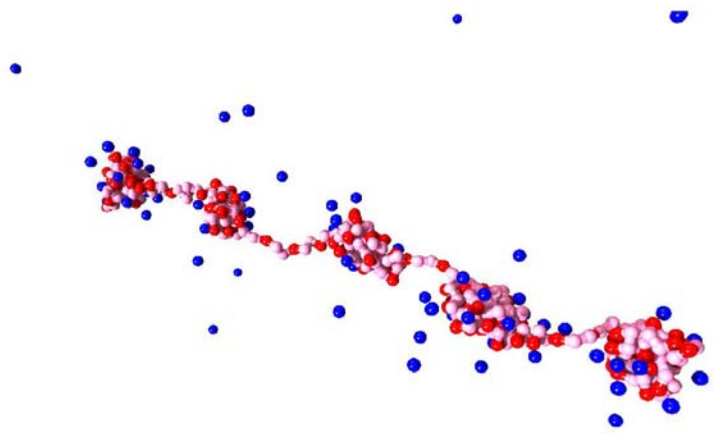
- What leads to shear localization (bands)?

Planned activities:

- molecular dynamics studies of both coarse-grained and atomistic models on the nanoscale: failure modes, conditions and mechanisms of localization, history dependence (aging), nonequilibrium steady shear
- connect to larger scales and longer times by using MD input in phenomenological models, test microscopic theories of flowing glasses

Electrostatic effects in (bio)materials

Pearl-necklace phase of polyelectrolyte



from: “Electrostatic effects in soft matter and biophysics”

- Charged systems pose major challenges to numerical simulation due to the long range Coulomb interaction
- We have developed local Coulomb algorithms based on auxiliary fields
- O(N) scaling
- Easy treatment of local dielectric effects

Planned activities:

• use the local algorithms to treat inhomogeneous dielectrics ε(r); contrast btwn. water (ε=80) and hydrocarbons (ε=2) often ignored.

• (re)examine in this context counterion distribution in front of charged surfaces (Guy-Chapman), like-charge attraction btwn. charged rods (DNA)

• long-term goal: improved mesoscale models for ion-channel transport