Multi-scale simulation of soft materials by using LAMMPS and OCTA/J-OCTA

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[Reference]
J. Chem. Phys., 117, 8153 (2002)

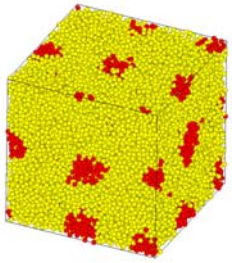
Summary

Molecular Dynamics (MD) of soft materials has to treat the long-time relaxation phenomena.

- Coarse Grained (CG) model
- Equilibrium (phase separated) structure by using the results of Self Consistent Field Theory (SCFT)
- Parallel MD simulation by using LAMMPS to calculate long-time relaxation and slow deformation

→ Effective simulation scheme for soft materials

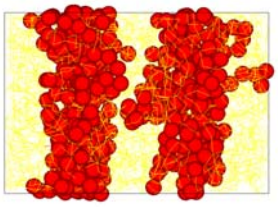
ABA tri-block copolymer (Thermo Plastic Elastomer) / Phase separated structure



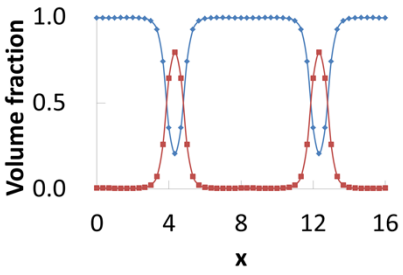
- Equilibrium Structure by using SCFT and DBMC
- Non-bond potential = LJ
  ε=1.0, σ=1.0
  r_{cut_off} = 2.5(Red/Red)
  1.5(Red/Yellow)
  $2^{1/6}$(Yellow/Yellow)
  → Red = hard segment
  Yellow = soft segment
- Bond potential = FENE
- Periodic boundary condition

Converter function of J-OCTA from COGNAC to LAMMPS

Density Biased Monte Carlo (DBMC) [OCTA-COGNAC]

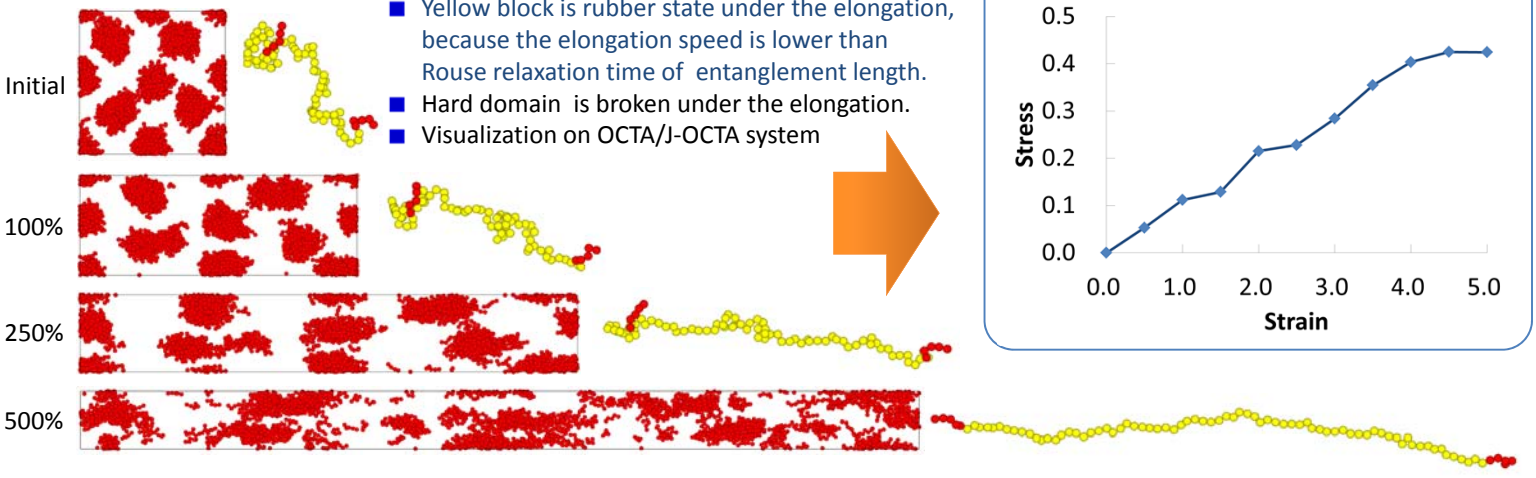


Self Consistent Field Theory (SCFT) [OCTA-SUSHI]



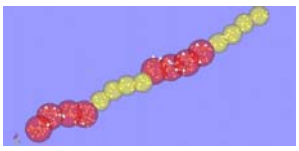
Elongation [LAMMPS]

- High speed parallel calculation
- Langevin Dynamics (Kremer-Grest model), T=0.4
- Yellow block is rubber state under the elongation, because the elongation speed is lower than Rouse relaxation time of entanglement length.
- Hard domain is broken under the elongation.
- Visualization on OCTA/J-OCTA system



Stress Strain Curve

Future Work



- CGMD with coarse grained potential obtained from atomistic model
- Comparison between experiment and simulation
- Other phase separated structures

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