Stress analysis in a patchy-particle based hydrogel simulation

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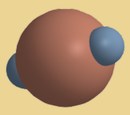
Description of the model

A polymer network is approximated using two types of patchy particles; monomers with two patches and cross-linkers with four patches. The patches are spheres of 0.2σ and are symmetrically positioned around a central particle with radius of 0.5σ. The position of the patches is fixed.

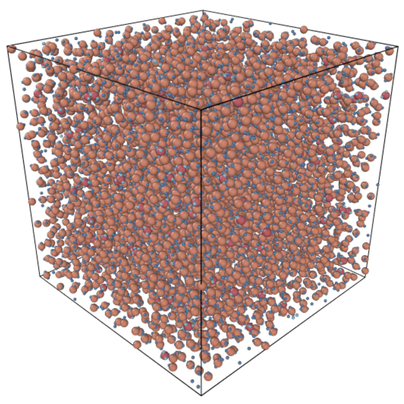
Cross Linker 

Monomer 

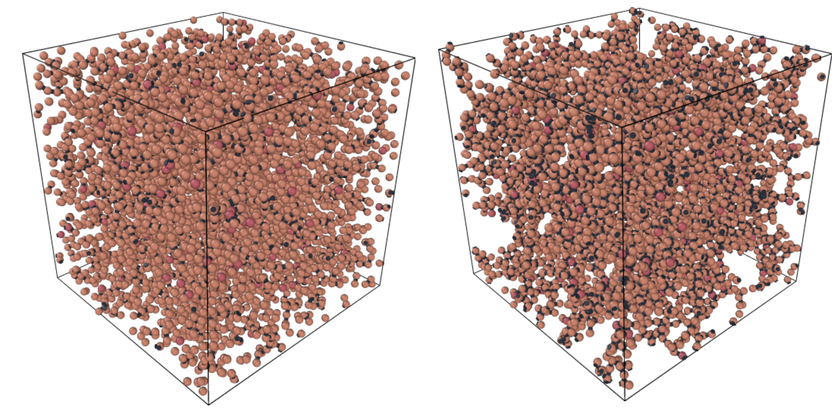
Simulation protocols

A set of two simulations in LAMMPS are performed first to approximate the polymer structures and then to apply a shear deformation. The simulation to approximate the polymer structures consists of a heating-up process and a isothermal process. Then, a shear deformation is applied in the xy plane with different shear rates. Finaly three successive deformations are applied, with constant relaxation periods between deformations.

Heat up

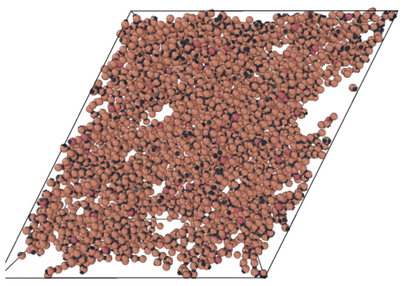


Isothermal

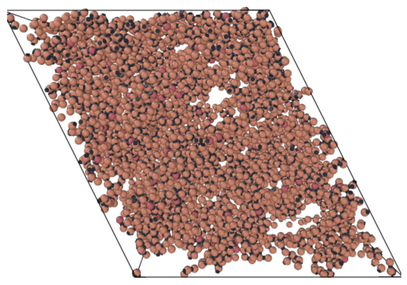


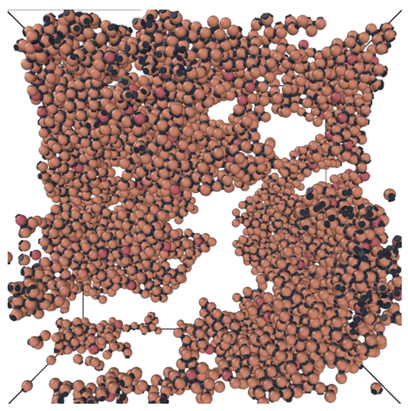
Shear deformation and relaxation intervals

Before flip



After flip





Conclusion

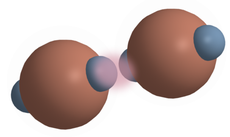
From the initial exploration of the relation between the yield stres-shear rate, we found a guide to classify the deformation behaviour through well-known models suchas as the Herschel-Bulkley model. On the other hand, from the set of deformation cycles with relaxation intervals between them we observe a stationary value of stress after the relaxation intervals.

In further explorations we want to find relations of the polymeric structure through different cross-linker concentrations at different shear rates to see how the yield-stress changes and compared them with the results from cycles of deformations with relaxation intervals.

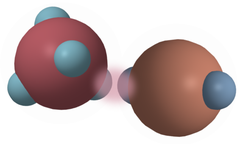
Interaction between patches

The central particles interact through a WCA potential, while the patches interact via an attractive potential and a three-body potential. The central particles and the patches do not interact with each other.

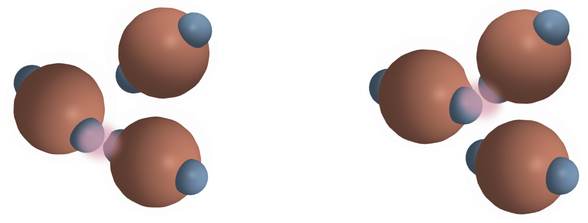
Patch B - Patch B

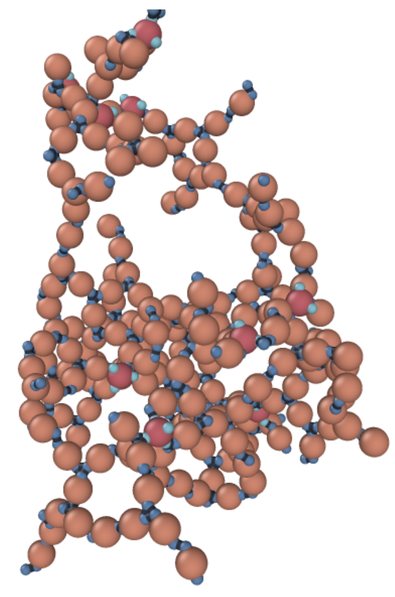


Patch A - Patch B



Swap Mechanism





Results

We report strain vs stress relation of shear deformation at different shear rates (Fig 1). Then, using the stationary stress values we construct a yield-stress curve (Fig. 2). Finally, we show the strain vs stress relation for each cycle (Fig. 3) and the stress of the system during the relaxation intervals between each cycle (Fig 4).

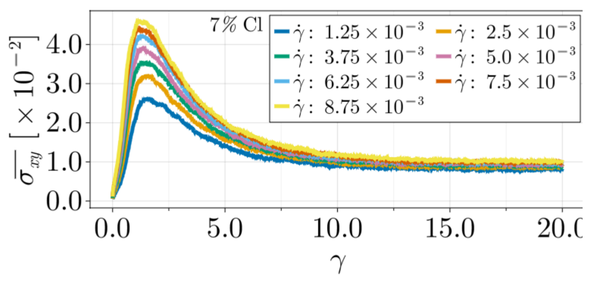


Figure 1: Stress vs strain

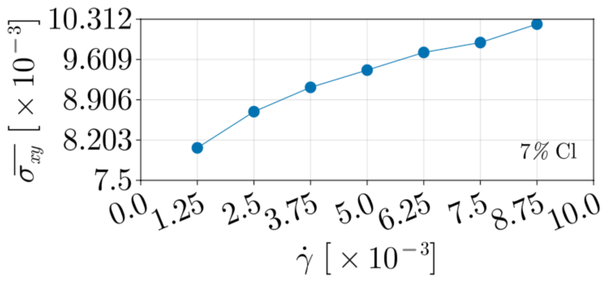


Figure 2: Stress vs shear rate

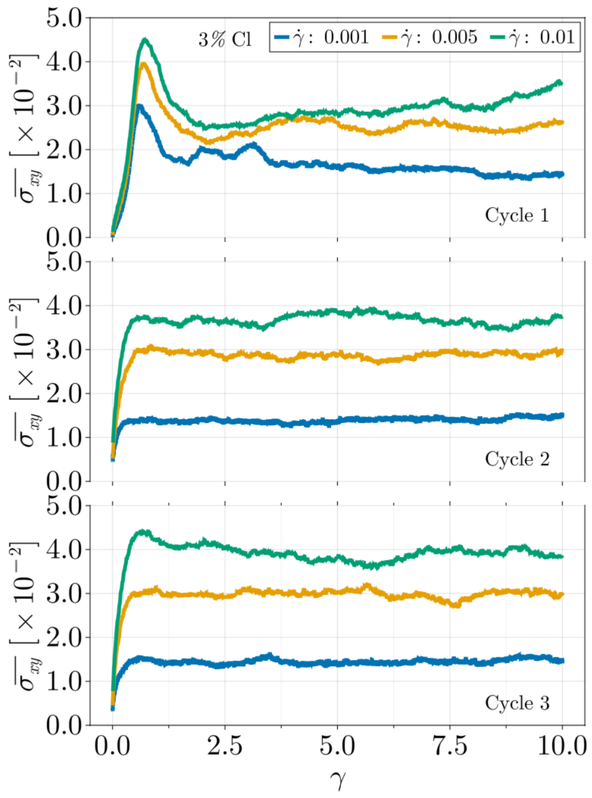


Figure 3: Stress vs strain cycles

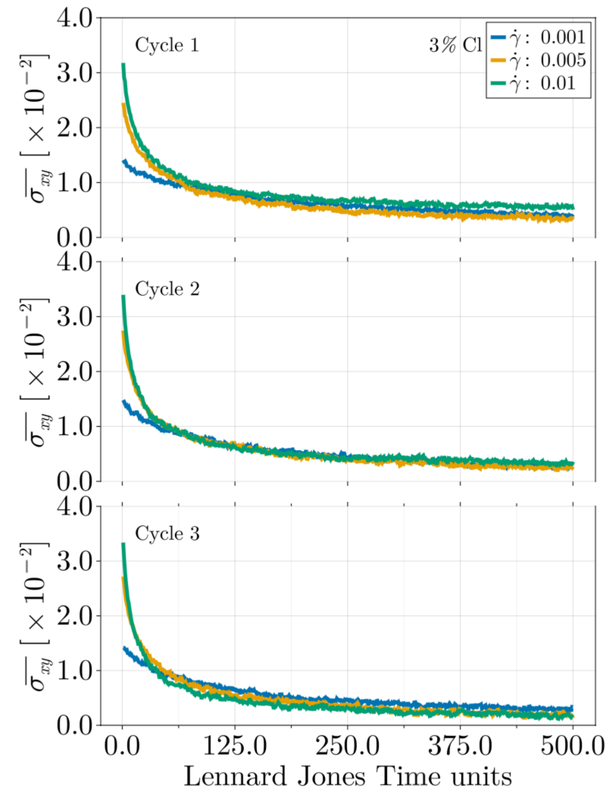


Figure 4: Stress vs relaxation time

References

[1] N. Gnan, L. Rovigatti, M. J. Bergman, and E. Zaccarelli, "*In Silico Synthesis of Microgel Particles*," Macromolecules, vol. 50, no. 21, pp. 8777–8786, Oct. 2017 [2] Valerio Sorichetti et al., "*Structure and elasticity of model disordered, polydisperse, and defect-free polymer networks*," The Journal of Chemical Physics, vol. 158, no. 7, Jan. 2023 [3] A. K. Subramaniyan and C. T. Sun, "*Continuum interpretation of virial stress in molecular simulations*," International Journal of Solids and Structures, vol. 45, no. 14–15, pp. 4340–4346, Jul. 2008