Stress analysis in a patchy-particles based hydrogel simulation.

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Abstract

Hydrogels can be effectively modeled as polymeric networks composed of monomers and cross-linkers. Over the past decade, a model system inspired by microgels particles methodologies using molecular dynamics has developed. This model system utilizes implicit liquid phase and a solid phase depicted by patchy particles. This study aims to investigate the relationship between the structure of polymeric networks and their mechanical response to shear deformation using a similar model system. The network structure is modified by varying the concentration of patchy particles that model the cross-linker, while the mechanical response is explored through two types of shear deformation simulation schemes: (1) constant shear deformations at various shear rates, and (2) constant deformations combined with relaxation intervals. Preliminary results from both simulations schemes indicate an initial overshoot in the components of the virial stress tensor parallel to the deformation direction. In the first simulation scheme, a yield-stress behaviour is reproduced in the steady-state of the deformation. In the second simulation scheme, increasing the concentration of cross-linkers amplifies the magnitude of the overshoot. Additionally, it is observed that when the relaxation time between deformations is equal to the deformation time, this overshoot reappears.

Keywords: Molecular dynamics, Patchy Particles, Hydrogels, Soft Colloids, Shear deformation

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