Simulation of Soft Magnetic Polymer Composites

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By combining magnetic nanoparticles and polymers, one obtains smart materials whose shape and elasticity can be controlled by an external magnetic field[1, 2]. They are of interest for applications such as actuation and transport both, in the technical and biomedical field. The latter is particularly relevant, as biological tissue tolerates magnetic fields. The interesting properties of magnetic gels rely on the combination of the magnetism of the nanoparticles and the elasticity of the surrounding polymer. The nature of this coupling is key to tailoring the material's responsiveness to external stimuli. Experimentally[3], the coupling is probed using AC susceptometry: the frequency-dependent response of the magnetic nanoparticles to an external AC magnetic field elucidates their interaction with their local environment.

In our contribution, we report on corresponding computer simulations[4, 5]. We obtain AC susceptibility spectra from simulations combining molecular dynamics and lattice-Boltzmann hydrodynamics. They are performed using the ESPResSo simulation package[6, 7]. In contrast to the experiments, in simulations, one can switch individual contributions to the polymer-nanoparticle coupling, such as van der Wals forces, covalent bonds, electrostatics and hydrodynamics. By switching them individually, we can study the effect of these interactions' effect on the magnetic susceptibility and other magnetomechanical properties.

References

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