Rheology and topology of a magnetic nanogel

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Magnetic nanogels (MNG) -- soft colloids made of polymer matrix with embedded in them magnetic nanoparticles (MNPs) -- are promising magneto-controllable drug carriers. In order to develop this potential, one needs to study MNG's behavior in various microfluidic systems, one of which can be modelled as a channel with a shear flow. At the same time, MNG motion can be governed by an external magnetic field, alongside with other factors, such as temperature, quality of the solvent or gels topology. The latter is usually controlled by spatial distribution of crosslinkers in the gels polymer matrix. Thus, a clear understanding of the interplay between magnetic, topologic and hydrodynamic influence on MNGs dynamics will be an essential step to facilitate their usage in targeted drug delivery [1].

Considering the size of the MNG and typical time and velocity scales involved in their nanofluidics, experimental characterisation of the system is challenging. In this work, we perform molecular dynamics (MD) simulations combined with the Lattice-Boltzmann (LB) scheme [2] aiming at describing the impact of the shear rate and applied magnetic field on the shape, magnetic structure and motion of an MNG with a given topology: uniform, with shifted centre of mass, with Gaussian distribution from the centre to periphery and reverse. An example of a simulated system shown in Fig. 1.

We find that in a shear flow, the centre of mass of an MNG tends to be in the centre of a channel and to move, preserving the distance to both walls. The MNG monomers along with translation are involved in two more types of motion, they rotate around the centre of mass and oscillate with respect to the latter. It results in synchronised tumbling and wobbling of the whole MNG accompanied by its volume oscillates. The fact, the MNG is a highly compressible and permeable for the carrier liquid. It makes its behaviour different from a simple droplet in an emulsion. We show that the volume oscillations and rotations are two faces of the same periodic process whose frequency is a growing function of the shear rate [3]. We find that the stronger magnetic interactions between MNPs are, the higher is the frequency of this complex oscillatory motion, and the lower is its amplitude. Finally, we show how this frequency depends on gels topology, external magnetic field and density of MNPs filling.

REFERENCES

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FIGURES

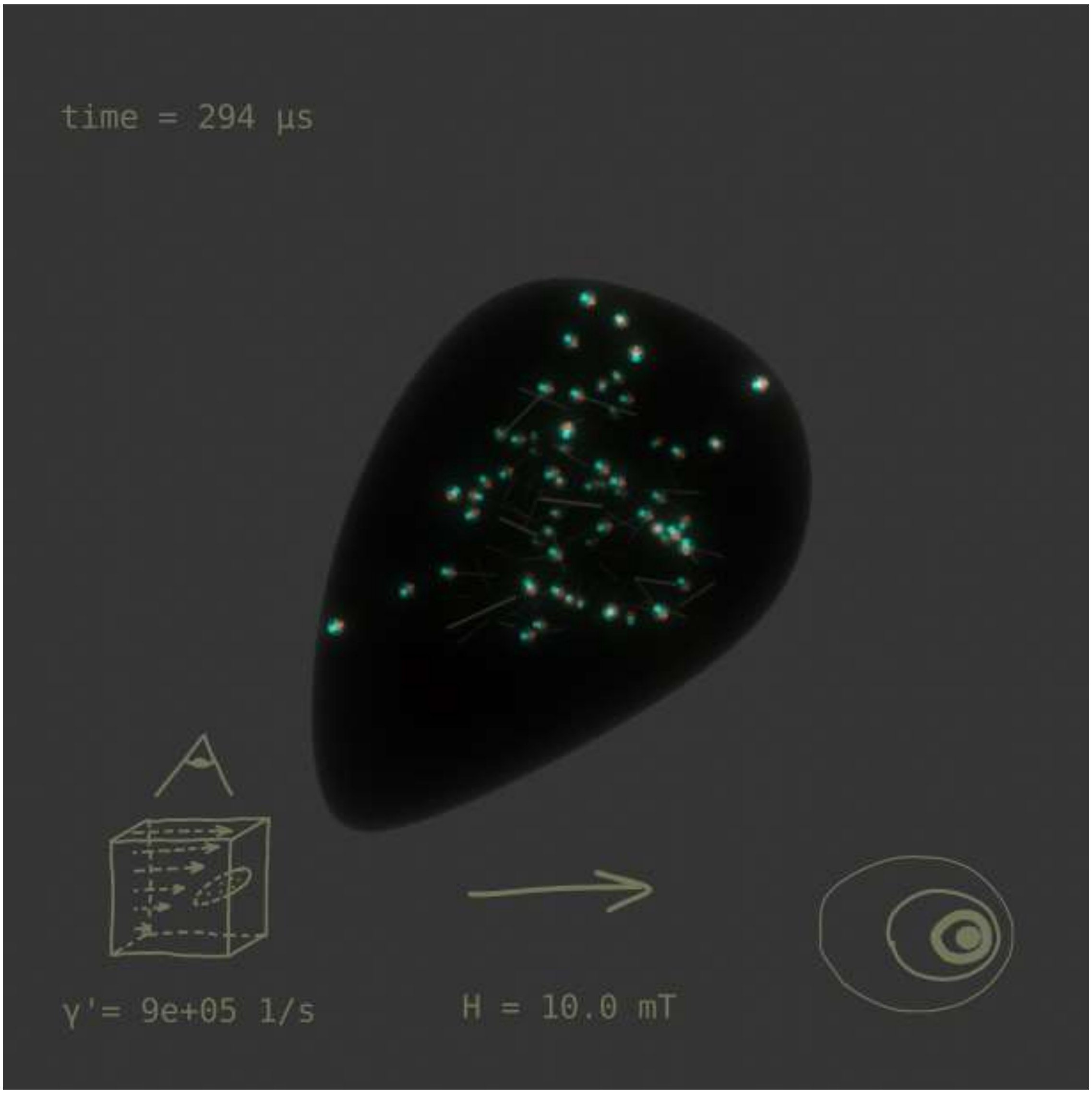

Figure 1: Simulation snapshot of an MNGs with shifted center of crosslinking in shear flow under and external magnetic field; arrows are MNPs and crosslinking bonds are represented by sticks.