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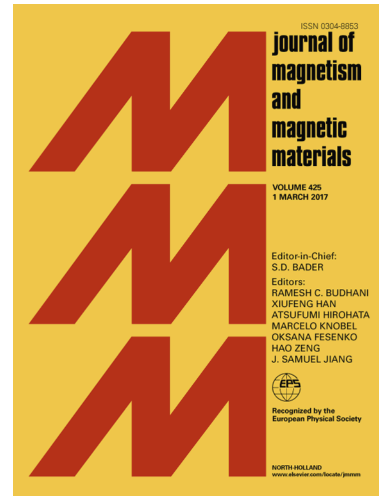

The influence of the magnetic filler concentration on the properties of a microgel particle: zero-field case

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The influence of the magnetic filler concentration on the properties of a microgel particle: zero-field case

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Abstract

In this contribution we present a molecular dynamics study of a microgel colloidal particle filled with magnetic nanobeads. The microgel is constructed of crosslinked polymer chains, some beads of which are magnetic. We vary the concentration of magnetic particles and the degree of crosslinking in the microgel to analyse the influence of both factors on the radius of gyration, microstructure and the initial magnetic susceptibility of our soft magnetic colloid. We show that even for a loosely crosslinked microgel, the concentration of magnetic filler must be rather high in order for the magnetic dipolar interactions to affect the shape and the internal structure of the soft colloid.

Keywords: Magnetic microgel, Ferrogel, Initial magnetic susceptibility, Computer simulations

1. Introduction

The combination of magnetic particles of nano- or/and micro-meter size and a polymer matrix gave rise to a new class of soft materials [1, 2, 3, 4, 5]. Among them, the most actively studied are magnetic gels, in which the polymer matrix is swollen by a carrier liquid [6, 7, 8, 9, 10, 11, 12, 13], and soft magnetic elastomers, also known as magnetorheological elastomers, that are magnetic rubber-like dry materials [5, 14, 15, 16, 17, 18, 19, 20].

Characteristic to these materials, the coupling between the magnetic interactions and the deformation of the polymer matrix makes them very promising for various technological applications, such as adaptive damping devices, vibrational absorbers, artificial muscles and many others [16, 21, 22, 23, 24, 25, 26]. However, despite the growing scientific and industrial interest that magnetic gels and elastomers are attracting, their properties are still far from being completely understood.

Magnetic gels and elastomers have been studied to date using different strategies. Computer simulations of these systems are usually based on coarse-grained approaches: magnetic particles are represented as beads with point magnetic dipoles, whereas the polymer matrix is either modelled implicitly [27, 28] or represented with different levels of detail [29, 30, 31, 32, 33, 34, 35, 36, 37, 38]. Along with computer simulations, several works employ continuum analytical theories [39, 40, 41, 42] to describe the magneto-elastic coupling of these materials.

Among magnetic soft materials, one class of the most novel and interesting systems are the ones known as microgel particles or soft colloids. These particles are formed by polymers crosslinked in a network whose size is of the order of 10 nm to 1 μm. The synthesis of microgels is usually based on polymerisation techniques with added crosslinkers [43, 44]. Crosslink density influences both the particle's internal structure and its swelling properties. Since swelling and deswelling are determined by the balance between the elastic forces of crosslinkers and the rest of interactions in the system, it can be controlled by different factors like, for example, temperature, solvent quality or, when the microgel particle carries embedded magnetic beads, external magnetic fields [43, 44, 45, 46, 47, 48]. This ability to change their size in response to external perturbations makes microgels advanced materials with potential for many applications [49, 50, 51, 52, 43]. In addition, self-assembly of concentrated microgels can be tuned by change or additionally imposed electric fields [53, 54, 55, 56]. In particular, microgels with embedded magnetic particles [45] are interesting materials from the point of view of both, technological applications and fundamental knowledge, and are the main subject of this work.

In this study we analyse the influence of interparticle magnetic interactions on the shape, microstructure and magnetic susceptibility of a microgel particle by means of computer simulations. We thoroughly study microgels with different degrees of crosslinking and containing different amount of permanently magnetised particles. We also vary the strength of magnetic interparticle interactions, analysing the effect of such parameters on the gyration radii of the microgels and their initial susceptibility. Finally, we also extract information about the formation of clusters of magnetic particles in the system.

The manuscript is organised as follows: In the next section we introduce the microgel model and our simulation approach. The main results are provided in Section 3. Finally, the summary of the work and the outlook can be found in Conclusions.

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