Monte Carlo and Experimental Study of the Magnetic Behaviour of Superparamagnetic Nanoparticles

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Superparamagnetic Iron Oxide Nanoparticles (SPION) are nanosize crystals of magnetite or maghemite. Their peculiar magnetic properties makes them particularly suited for a variety of biomedical applications, ranging from cellular imaging to cancer treatment by hyperthermia [1]. The usual theory used to describe their magnetic behaviour is that developed by Paul Langevin [2], which only applies to idealized (isotropic, monodisperse in size and non-interacting) nanoparticles at high temperatures. Reality however always deviates from that theoretical framework: real samples exhibit polydispersity in sizes, particles usually have at least one anisotropy axis, and, particulary in biological media, they tend to aggregate, leading to locally high particle volumic fractions and therefore interaction between their magnetic moments [3]. All those phenomena impact the magnetization of particle ensembles in a non-trivial way and are impossible to model simultaneously theoretically.

In this work, these deviations from the Langevin law are studied numerically, at thermodynamic equilibrium and at 300K, using a Metropolis algorithm, and compared with experimental data obtained using a Vibrating Sample Magnetometer for real SPION, whose size distribution was evaluated by transmission electron microscopy. Thorough tests are led on the simulations to ensure convergence of the magnetization. The effect of each parameter on the field-dependent magnetization curves is then studied.

Figure 1 shows an example of the impact of one of those parameters: inhibiting rotation of the particles (i.e. the Brown relaxation process). As can be seen, it leads to a slower saturation of the magnetization in samples with a high size dispersion parameter ($\sigma_L = 0.5$). Likewise, the presence of dipolar interaction between particles also leads to slower saturation in such samples, as does drying samples under a magnetic field perpendicular to the measurement field (as opposed to drying them under a field parallel to the measurement field, which yields the opposite effect). These various modifications of the curves result in erroneous size dispersion parameters when fitting them to an integrated Langevin equation. The simulations compare well with experimental results, as can be seen on figure 2. In future work, the simulations could be improved by changing the anisotropy model from uniaxial to a more realistic cubic anisotropy.

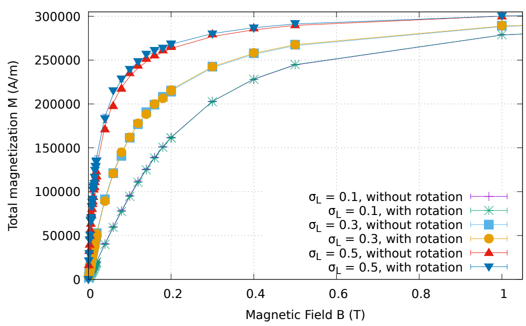

Fig. 1 Impact of the particles' ability to rotate on the magnetization curve of particles with a lognormal distribution of their radii, a 3nm median radius and varying size dispersion parameters ($\sigma_L = 0.1, 0.3, 0.5$.

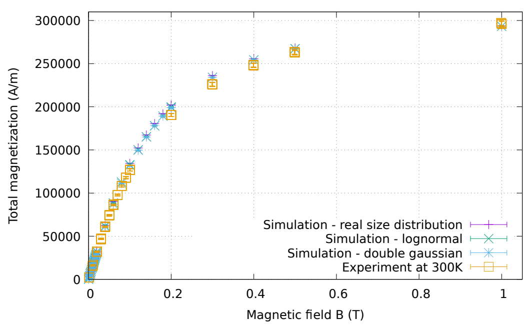

Fig. 2 Comparison between experimental results (in orange) obtained on HiQ Nano 6nm maghemite nanoparticles, and three simulations differing in the particle size distribution.

References

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