Modelling of magnetic nanoparticle clusters and effects on hyperthermia properties

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In the last decade, magnetic nanoparticles (MNPs) made of iron oxides have been intensively studied for potential application in cancer therapies based on magnetic hyperthermia [1,2]. The magnetic behaviour and the hysteresis losses of isolated magnetic nanoparticles are well described by micromagnetic analytical models. However, the energy losses predicted by such models only loosely provide an estimation of the magnetic nanoparticle specific loss power (SLP), which is usually derived from thermometric or calorimetric measurements in quite different experimental conditions, used for hyperthermia modelling [3]. It is indeed very difficult to include the effect of magnetostatic dipole-dipole interactions into analytical models, when the particles are randomly clustered, leading to a non-accurate evaluation of their heating properties. Hence, the need to solve the Landau Lifshitz Gilbert equation with a numerical approach to study the influence of MNP clustering on SLP, as well as the dynamic response to different exciting magnetic fields. Numerous 3D numerical codes have been proposed [4]. These solvers can study very complex magnetic nanostructures, however, are computationally very intensive and not suitable to describe thousands of interacting nanoparticles. To this aim, following the macrospin approach of Haas and Nowak [5], we developed a numerical solver where the magnetization dynamics of each mono-domain MNP is modelled as a single magnetic moment, following the LLG equation, including the dipole-dipole interactions, and the thermal effects, using the Langevin dynamics.

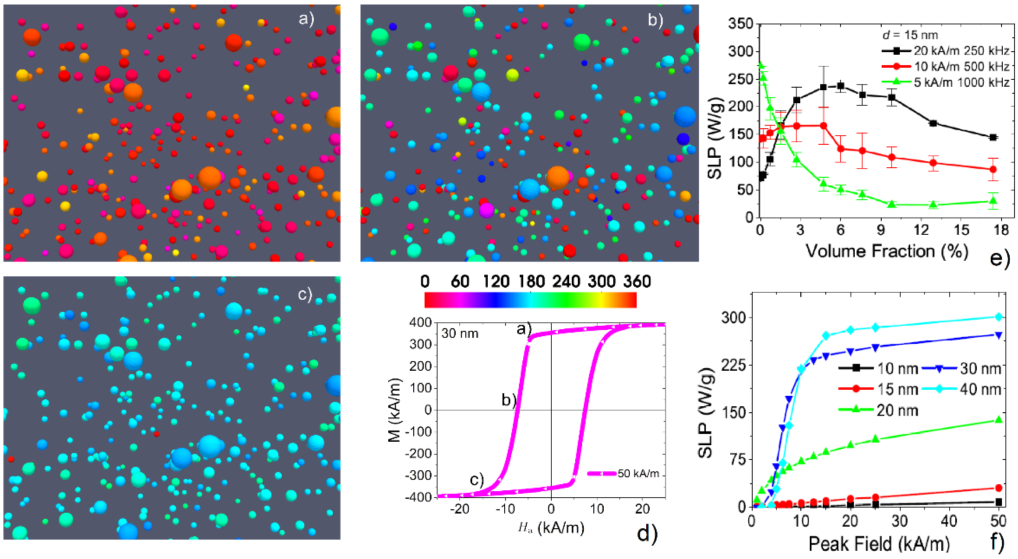

Figure 1: Snapshots of the angle between the magnetization and the positive direction of the applied field for a stochastic distribution of NPs with a diameter of 30 nm in the non-interacting approximation. a) Descending hysteresis branch, before the magnetization reversal, b) Ha=Hc, c) descending hysteresis branch after the magnetization reversal, d) Corresponding calculated Hysteresis loop. e) SLP as a function of Volume fraction, calculated for clusters of NPs with an average size of 15 nm for different exciting magnetic fields, f) SLP calculated for diluted MNPs of different sizes, ad function o f the peak field amplitude.

References

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