

Monte Carlo Simulations of the T₂ relaxivity induced by Cubic Shaped Superparamagnetic Nanoparticles

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Superparamagnetic iron oxide nanoparticles (SPION's) are nanoscale particles mainly composed of magnetite or maghemite. They are characterized by a unique combination of small size, high surface area-to-volume ratio and a high saturation magnetization at 300K, which makes them useful for a variety of biomedical applications [1] such as magnetic resonance imaging (MRI), hyperthermia therapy, drug delivery, ...

The contrast between a zone of interest and its surrounding tissue is an important aspect of MRI images. A higher contrast allows a clearer and an easier diagnosis. MRI contrast depends on the longitudinal (T₁) and transversal (T₂) relaxation times : These are characteristic times for the system to return to equilibrium after a magnetic excitation pulse. SPIONs are used as contrast agents that are targeted to the tumor and darken the tumor on the MRI image.

In this work, the effect of cubic shape nanoparticles on the transverse relaxation time (T₂) at high magnetic field and at 300K is studied via Monte Carlo methods. A CPMG sequence was simulated via a well-known methodology from reference [2]. The magnetic field generated by a cubic particle has been numerically computed with COMSOL. We simulate cubes and spheres over a range of sizes (from 20 to 500 nm). Relaxation times between cubes and spheres can be compared at equal volume in order to maintain the same magnetic moment for both shapes. The diffusion of protons is modeled by a random walk, their spins as vectors and the dephasing arises from the rotation of the spin around the local magnetic field inhomogeneities over time.

Our preliminary results indicate that there is no significant differences between the transverse relaxation times (T₂) associated to the cubic and spherical shaped particles in the static regime and the partial refocusing regime. Our future work will study the influence of nanoparticle shapes inside the motional average regime (MAR) for other shapes (stars, cylinders, ...) and the effect of aggregation on the transversal relaxation time (T₂).

References

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- [2] V. Quoc Lam, P. Gillis and Y. Gossuin, "Monte Carlo simulation and theory of proton NMR transverse relaxation induced by aggregation of magnetic particles used as MRI contrast agents", in *Journal of magnetic resonance*, 2011, vol. 212, pp. 139-148