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MONTE CARLO SIMULATIONS OF THE T2 RELAXIVITY INDUCED BY CUBIC SHAPED SUPERPARMAGNETIC NANOPARTICLES

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Nanoscale materials have garnered immense attention in the scientific community for the past few decades due to their wide range of applications [1] and their unique properties. At this scale, magnetite and maghemite particles exhibit superparamagnetic behavior at room temperature in addition to a high surface area-to-volume ratio. SuperParamagnetic Iron Oxide Nanoparticles (SPIONs) are predominantly used as T_2 and T_2^* contrast agents to detect tumors in Magnetic Resonance Imaging (MRI) [1]. When SPIONs are introduced inside a tumor by targeting methods, the associated T_2 is decreased which darkens the tumor on the MR images.

Usually, SPIONs particles are synthetized in a spherical shape. However, over this last decade, some studies synthesized exotic-shaped particles [2] and measured a decrease in T_2 by a factor 2 or even more compared to the usual spherical-shaped SPIONs. In our work, we propose to assess the impact of SPION's shape on T_2 using relaxation simulation and an analysis of the stray field of a cubic-shaped SPION.

NMR CPMG sequences were simulated using a well-known Monte Carlo method considering cubic and spherical SPIONs under a very high magnetic field B_0[3]. The magnetic stray field of a cubic particle is analytically derived from the demagnetization tensor field [4]. Proton diffusion is modeled by a random walk considering a water diffusion coefficient at 300°K. Each proton spin is represented by a vector in the plane perpendicular to B_0.

Our results indicate that there are no significant differences between cubic and spherical shaped SPIONs when their diameters are larger than 30 nm, corresponding to the Static Diffusing Regime (SDR) and over 200 nm in the Partial Refocusing Regime (PRR). However, in the Motional Average Regime (MAR), i.e. for particle sizes smaller than 30 nm, a 10 to 20% decrease in T_2 is observed for cubic SPIONs compared to spherical SPIONs. To quantitatively interpret these results, NMR relaxation models, which include an analysis of the field distribution, were applied to the two shapes [5] [6]. These models confirm our simulation results in the three regimes.

[1] A. Ito, M. Shinkai, H. Honda, T. Kobayashi *Journal of Bioscience and Bioengineering.* **100**, 1-11 (2005)
[2] R.G.D. Andrade, S.R.S. Veloso, E.M.S. Castanheira *International Journal of Molecular Sciences.* **21**, 2455 (2020)
[3] Q.L. Vuong, P. Gillis, Y. Gossuin *Journal of Magnetic Resonance.* **212**, 139-148 (2011)
[4] S. Tandon, M. Beleggia, Y. Zhu, M. De Graed *Journal of Magnetism and Magnetic Materials.* **271**, 9-26 (2004)
[5] S. Majumdar, J.C. Gore *Journal of Magnetic Resonance*. **78**, 41-55 (1987)
[6] R.J.S. Brown *Physical Review.* **121**, 1379-1382 (1961)