Monte Carlo Simulations of the T_2 relaxivity induced by Exotic-Shaped Superparamagnetic Nanoparticles

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Nanoscale materials have garnered immense scientific interest over the past few decades due to their wide range of applications [1] and their unique properties, such as enhanced surface reactivity and quantum effects. Among them, SuperParamagnetic Iron Oxide Nanoparticles, typically composed of magnetite and maghemite, exhibit superparamagnetic behaviour at room temperature and possess a high surface area-to-volume ratio. These properties make SPIONs particularly valuable as T_2 or T_2^* contrast agents in Magnetic Resonance Imaging (MRI) for tumour detection. By reducing the transverse relaxation time (T_2) within targeted tumour tissues, SPIONs enhance image contrast between healthy and diseased regions, thereby improving diagnostic accuracy.

In this work, we investigate how the shape of SPIONs influences transverse relaxation T_2. Relaxation was modelled by Monte Carlo simulations of CPMG sequences using nanoparticles ranging from 10 to 600 nm in diameter [2, 3]. The relaxivities $(1/T_2)$ of anisotropic shapes (cubes, cylinders and tetrahedra) were compared, volume-wise, with those of spheres. Furthermore, we propose a methodology [3] to predict the impact of arbitrary shapes on relaxation time based on Monte Carlo analysis of their magnetic stray field.

Contrary to prior experimental reports [4], our results indicate that relaxivity $(1/T_2)$ is not significantly impacted by particle shape. Only nanoparticles smaller than 30nm, in the motional average regime, show measurable differences, with some shapes exhibiting up to a 15% increase and others up to a 30% decrease.

References

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