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

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Nanoscale materials have garnered immense scientific interest for the past few decades due to their wide range of applications [1] and their unique properties, such as enhanced surface reactivity and quantum effects. At this scale, composite materials of magnetite and maghemite exhibit superparamagnetic behavior at room temperature in addition to a high surface area-to-volume ratio. Those superparamagnetic iron oxide nanoparticles (SPION) are predominantly used as T2 or T2* contrast agents to detect tumors in magnetic resonance imaging (MRI) [1]. In MRI, the image quality is closely tied to the enhancement of contrast between two distinct tissue types. To artificially increase the contrast, SPION can be introduced inside the tumors via targeting methods to reduce the transversal relaxation time (T2), making the tumor appear darker on images.

In this work, the effect of the SPION shape [2] on T2 is theoretically studied in a high magnetic field at room temperature. Monte Carlo simulations of CPMG sequences using cubic nanoparticles ranging from 20 to 500nm have been simulated via a well-known methodology from reference [3]. The analytical magnetic stray field of cubic particles is implemented [4], and results are compared volume-wise to spherical particles to keep the magnetic moment constant. The diffusion of protons is modeled by a random walk and their spins as vectors rotating around the stray field of the cubic particles.

Our results indicate that the transverse relaxation time does not significantly change between a cubic particle and a spherical particle for sizes over 20 nm, corresponding to the static diffusion regime and the partial refocusing regime. For particles below the 20 nm threshold, corresponding to the motional average regime (MAR), a 10% increase in T2 is observed for the cubic nanoparticles.

References

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