Monte Carlo Simulations of the T_2 relaxation induced by Cubic Shaped Superparamagnetic Nanoparticles

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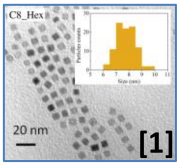
Theoretical analysis of water protons transverse relaxation (T_2) induced by cubic-shaped superparamagnetic nanoparticles (Np) of magnetite, used as negative contrast agents in MRI, has been conducted with Monte Carlo simulations considering a high static magnetic field (B_0). The comparison between spherical and cubic-shaped nanoparticles, at equal volumes, revealed minor deviations in the transverse relaxation (T_2) within the Motional Average Regime [d < 30nm] whereas no deviation was observed for larger particles [d > 30nm].

I. Introduction and research context

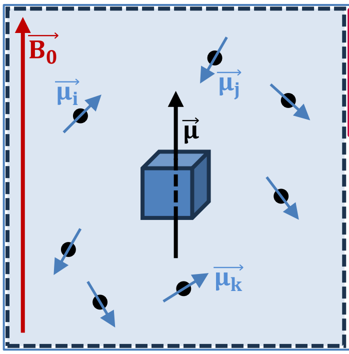
- For the last 20 years, there has been an ongoing interest in the synthesis and characterization of non-spherical nanoparticles. Several experimental studies, such as [1], using exotic particles reported an increase in the efficiency of shortening water relaxation times T_1 and T_2.
- In contrast, very few studies have confronted experimental results to simulations or theory. Our goal is to study the influence of non-spherical shape induced relaxation by magnetite nanoparticles using Monte Carlo simulations.



[1]

II. Methodology

II. a. Simulation Setup [2]

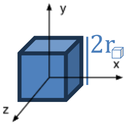


- 10 000 Protons ●
  - $\Longrightarrow$ Each with spin, $\mu_i \hat{e}_{xy}$
- 1 Cubic Np
  - $\Longrightarrow$ Magnetic Moment, $\mu\hat{e}_z$

- Static Magnetic Field, $B_0\hat{e}_z$
- Proton Diffusion via Random Walk
- CPMG Sequence, $T_E \sim \mathrm{ms}$
- Periodic Boundaries – – –

$\Longrightarrow$ Uniformly distributed Np's in aqueous solution

II. b. Simulations



Analytical Magnetic Field for a cubic particle [3]

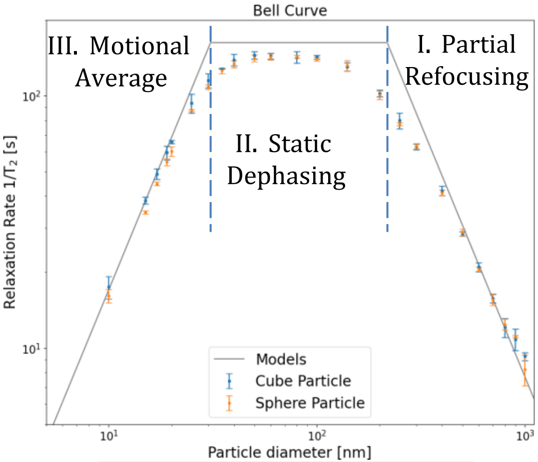
$$\begin{cases} x_k = x + (-1)^k r_{\square} \\ y_l = y + (-1)^l r_{\square}, \\ z_m = z + (-1)^m r_{\square} \end{cases} \qquad r_{klm} = \sqrt{x_k^2 + y_l^2 + z_m^2}$$

$$\Longrightarrow B_z = \left(\frac{\mu_0 M_0}{4\pi}\right) \sum_{k,l,m=0}^{1} (-1)^{k+l+m} \operatorname{arctg}\left(\frac{x_k y_l}{z_m r_{klm}}\right)$$

Temporal evolution of proton spin $\phi(\vec{r}(t))$:

- $\vec{\mu}_{i\perp}(t) = \mu^0_{i\perp}(\cos(\phi),\ \sin(\phi))$
- $\vec{\mu}_{i\parallel}(t) = \mu^0_{i\parallel}$
- $\Delta\phi(\vec{r}(t)) = \gamma B_z(\vec{r})\,\Delta t \Longrightarrow$ Larmor precession $\omega_0(t) = -\gamma B_z(\vec{r})$
- $|<\vec{\mu}_\perp(t)>| \propto \exp(-t\,/\,T_2)$

III. T_2- Comparizon between spherical and cubic contrast agents



- I. II. No significant variations observed
- III. ~ 10% increase of $1/T_2$

I. Partial Refocusing (PR) Regime, [d > 200nm]

- Protons diffusing close to the Np are almost immediately lost from the signal due to high magnetic field gradients.

$\Longrightarrow$ Relaxation arises mainly from proton diffusion far from the Np.

- As the distance grows, the magnetic field of a cubic shaped Np converges to the magnetic field of a spherical Np.

$\Longrightarrow$ Proton spin dephasing in the PR is the **same for any shape**.

- It has been shown in [4] that $[1/T_2 \propto \sigma^2]$, where $\left[\sigma^2 = \frac{1}{V}\int \left|\vec{\nabla} B_z\right|^2 dV\right]$. Study of cubic shape Np $\sigma^2_{\square}$ showed a steep convergence as the distance from its center grows to the spherical Np $\sigma^2_{\circ}$; confirming our interpretation.

II. Static Dephasing Regime, [30nm < d < 200nm]

- The statistical distribution of the magnetic field $[P(B_z)]$ converges rapidly as the distance grows to the dipole model. The lack of variation in relaxation can then be explained by the relation $[1/T_2 \propto p(B_z)]$[5].

III. Motional Average Regime, [d < 30nm]

- Protons diffusing near the Np can perceive the contrast agent shape due to the small magnetic field intensity of the Np.
- Study of $[<B_z^2>]$ indicated a ~20% variation with the dipolar model which can be linked to our results via $[<B_z^2> \propto 1/T_2]$ by the Redfield theory.

IV. Summary and Future Directions

- Monte Carlo simulations demonstrate that the contrast agent shape has no impact on T_2 within the static diffusing and partial refocusing regimes. However, a 10% increase is observed in the Motional Average regime [d < 30nm].
- Future studies will focus on the agglomeration of exotic-shaped Np (stars, cylinders, …) and their impact on T_2 in the MAR.

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