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In search of multifunctional magnetic nano-particle design with micromagnetic simulations

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Abstract

Magnetic nanoparticles (MNP) serve as imaging tracers, therapeutic heating agents and biosensors in biomedical applications. All the above applications rely upon the particles' unique relaxation mechanisms, which lead to phase shifts in alternating magnetic fields and dissipation. As MNP have an intrinsic size distribution and their magnetic properties are also size-dependent, search is ongoing for the optimally sized MNP that could potentially serve for all three applications simultaneously. In this work, we present our current results on simulating the influence of core size, mono- and polydisperse size distributions as well as magnetic anisotropy on the performance of MNP for both heating and biosensing using micromagnetic dynamic magnetization simulations.

I. Introduction

Magnetic nanoparticles (MNP) serve biomedical applications as tracers for magnetic particle imaging (MPI), heating agents in magnetic fluid hyperthermia (MFH) and markers in biosensing. Among biosensing methods, dual-frequency magnetic particle spectroscopy (MPS), also termed frequency mixing magnetic detection (FMMD), enhances immuno-assays by introducing frequency mixing terms that provide additional information about the MNP sample. Concurrently, heat generated in MNP subjected to high frequency alternating magnetic fields (AMF) allow therapy with MFH or enhancing FMMD-based immunoassays by stimulating 1) binding or bond-breaking reactions and/or 2) antibody modification to enhance signal and improve limit of detection of immunoassays [1]. As we could recently show, FMMD [2] and MFH [3] performance strongly depends on MNP core size and magnetic anisotropy, whose influence on the MNP relaxation process is capably modeled using micromagnetic simulations [4], predicting stronger signal for larger sizes while indicating weaker dependency on magnetic anisotropy.

We present current findings on predicting MNP performance as biosensors in FMMD and heating agents in MFH, dependent on core size and anisotropy, using micromagnetic simulations, in search of potential MNP designs that enable thermo-regulated immunoassays with FMMD.

II. Methods and materials

Using micromagnetic simulations [4] we generated the magnetic response of 1000 Fe_3O_4-MNP (properties M_s = 476 kAm^{-1}, T = 300 K, MNP concentration $c = 10^{15}$ m^{-3}) to both dual- and single-frequency AMF, simulating

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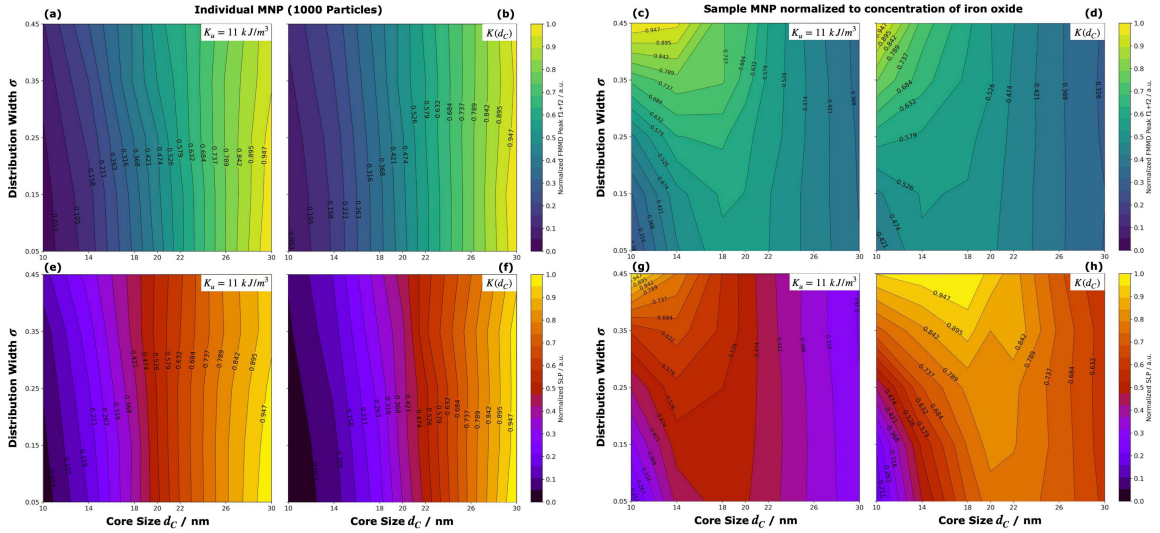

Figure 1: Mapping of performance parameters for FMMD (a-d) and MFH (e-h) for MNP of core sizes $d_C = (10,\ldots 30) nm$, ranging from mono- ($\sigma = 0.05$) to polydisperse ($\sigma = 0.45$). Simulations performed with constant (bulk) anisotropy K_u (a,c,e,g) or $K(d_C)$ (b,d,f,h). Data shown as individual MNP contribution ((a,b),(e,f)) or normalized to the concentration (amount) of Fe_3O_4 ((c,d),(g,h)).

FMMD (1) and MFH (2):

$$H_{FMMD}(t) = H_1 \sin\left(2\pi f_1 t\right) + H_2 \sin\left(2\pi f_2 t\right) + H_0\,, \quad (1)$$

where $f_1 = 2$ kHz, $H_1 = 1.2$ mT/μ_0, $f_2 = 40$ kHz, $H_2 = 16$ mT/μ_0 and $H_0 = (0,1,2,\ldots,24)$ mT/μ_0.

$$H_{MFH}(t) = H_0 \sin\left(2\pi f_0 t\right)\,. \quad (2)$$

where $f_0 = 250$ kHz, $H_0 = 25$ mT/μ_0. All AFM parameters represent typical experimental values.

We simulated M(H)-loops for core sizes of d_C = (10, 14, 18, 20, 22, 26, 30) nm with size-distribution widths of $\sigma = (0.05, 0.15, 0.25, 0.35, 0.45)$, thereby probing mono- to polydisperse MNP samples. The hydrodynamic size was kept constant at 100 nm. Magnetic anisotropy was assumed uniaxial with bulk value, K_u = 11 kJ/m^3, however, as it is also suggested to be inversely proportional to d_C, we also simulated its contribution according to [2]:

$$K(d_C) = K_u + \frac{6}{d_C} \cdot K_S, \quad (3)$$

with surface anisotropy assumed as $K_S = 50\ \mu J/m^2$.

III. Results and discussion

From M(H_{FMMD})-loops we calculated the signal intensity of the frequency mixing term, f_1+f_2, and extracted its peak value, $A^{\max}_{f_1+f_2}$, as a measure of FMMD performance [2]. From the area enclosed by each M(H_{MFH})-loop, we calculated the specific loss power (SLP) as a measure of MFH performance [3].

Both $A^{\max}_{f_1+f_2}$ and SLP values increase for increasing core sizes, as shown in Figure 1((a,b)&(e,f)). Notably, this trend is observed similarly for both simulating with $K_u = 11$ kJ/m^3 and $K(d_C)$ (cf. eq. (3)), except that when using K_u, the performance values maximize more towards monodisperse ($\sigma = 0.05$) rather than polydisperse MNP ($\sigma = 0.45$). These results suggest that individual MNP contribute the better to FMMD signal / MFH heating, the larger their core sizes are, as confirmed previously [2,3]. Here, the core size effect is dominating the effect of magnetic anisotropy.

As we simulate 1000 individual particles in constant volume, the amount of material (Fe_3O_4 concentration) increases with d_C. Normalizing results to concentration yields Figure 1((c,d)&(g,h)): Here, $A^{\max}_{f_1+f_2}$ and SLP values peak at $d_C \approx (15-20)$ nm for monodisperse MNP and at $d_C \approx (10-13$ nm for polydisperse MNP for $K_u = 11$ kJ/m^3. Interestingly, for $K(d_C)$, this trend is amplified for FMMD performance, peaking at $d_C \approx 10$ nm, but SLP values maximize at $d_C \approx (15-20)$ nm and show a relative increase by $\approx 50\%$ compared to K_u at equal values of d_C and σ. This indicates the importance of considering size-dependency of magnetic anisotropy.

IV. Conclusion

Our study of MNP core size, its distribution and magnetic anisotropy driven effects on particle detectability (FMMD) and heating (MFH) suggests best individual performance from largest particles. For samples of equal Fe_3O_4 concentration, however, smaller ($d_C \sim 15$ nm) and polydisperse MNP perform best and anisotropy does play

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a significant role. We plan to complement this study with simulated MPI data for further multifunctionality analysis towards theranostic applications.

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Author's statement

Authors state no conflict of interest.

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