Defect-engineering of bi-magnetic iron-oxide nanoparticles for optimal heating power

M. Vasilakaki[1], G. Antonaropoulos[2], E. Valamontes[3], A. Lappas[2], K. N. Trohidou[1]
[1]*Institute of Nanoscience and Nanotechnology, NCSR 'Demokritos', 15310 Athens, Greece*
[2] *Institute of Electronic Structure and Laser, Foundation for Research and Technology, Greece*
[3] *Dept. Electrical & Electronics Eng., University of West Attica, Athens, 12244, Greece*
m.vasilakaki@inn.demokritos.gr

Iron-oxide nanoparticles commercially used in biomedical applications show poor heating performance and MRI signals because of their low saturation magnetization and magnetocrystalline anisotropy. Defect-engineering combined with bi-magnetic core/shell morphology is proposed as an alternative pathway to improve the magnetic properties of these iron oxide nanoparticles [1].
In this study, we have investigated the magnetic effect of the atomic-scale defects, regarding vacant metal-ion crystallographic sites, in pure spherical core/shell $Fe_xO/Fe_{3-\delta}O_4$ and when substituting Co (12%-35%) in spherical core/shell $Co_yFe_{1-y}O/Co_xFe_{3-x}O_4$ nanoparticles [2]. We perform Monte Carlo simulations with the implementation of the Metropolis algorithm to investigate the cooling field dependence of the exchange bias and the coercive field at low temperature and we calculate theoretically the heating loss parameter due to susceptibility losses [3] in these systems. Our results demonstrate that the defects act as pinning centers resulting to a competition amongst the magnetic moments, resulting in turn in the non - coherent reversal and consequently to non-easy relaxation of the spins. This mechanism enhances the magnetic anisotropy of the defected system leading to a ten-fold increased heating performance comparing to that of the defect-free nanoparticle. The addition of a moderate percentage of Co substitution (~10%) together with a small well-preserved highly defected rock salt core and a large as less defective as possible spinel shell play a key role in improving almost 3 times the magnetically-mediated heating efficacy of the pure core/shell particle.
Our study highlights how structural and morphological characteristics can affect materials' design parameters to improve the iron-oxide based nanoparticles' magnetic heating performance.

[1] A. Lappas et al. Physical Review X, 9(4) (2019) 0410441
[2] G. Antonaropoulos et al. Nanoscale, 14 (2022) 382 – 401
[3] M. Vasilakaki et al. Nanoscale, 7 (2015) 7753-7762