XXXII Panhellenic Conference on Solid State Physics and Materials Science
Conference Center "Carolos Papoulias", 18-21 September 2016, Ioannina, Greece

Monte Carlo Study of core/shell nanoparticles for enhanced hyperthermia performance

M. Vasilakaki[1], K. N. Trohidou[1], G. Margaris[1], C. Binns[2]
[1] *Institute of Nanoscience and Nanotechnology,NCSR Demokritos,Aghia Paraskevi,Greece*
[2] *Department of Physics and Astronomy, University of Leicester, Leicester LE1 7RH,UK*

Abstract: Magnetic particle hyperthermia, namely the heating dissipation of magnetic nanoparticles (NPs) when exposed to an alternating magnetic field, is a promising cancer treatment technique with minima side effects. Active research is carried out to improve hyperthermia performance of NPs. The most studied and commercially produced colloids for magnetic hyperthermia contain iron oxide NPs. Recently, it has been demonstrated experimentally that complex nanoparticles Fe/Fe_3O_4 of core/shell morphology give higher SAR values than the single-phase oxides. [1]
We investigate theoretically the mechanism of magnetic hyperthermia due to susceptibility losses (SAR) in complex ferromagnetic (FM) core/ ferrimagnetic (FiM) shell nanoparticles. We use the Monte Carlo simulations technique with the Metropolis algorithm to simulate the magnetisation behaviour of complex FM/FiM nanoparticles of different core sizes and shapes. We calculate the magnetisation and we use our results in a modified linear Néel-Brown relaxation model [2] to calculate the SAR of Fe/ Fe_3O_4 nanoparticles.
Our calculations show that for all the sizes and shapes the complex FM/FiM nanoparticles give higher SAR values than the pure ferrimagnetic ones due to their higher core saturation magnetisation. Our results have the same characteristics as the available experimental data from Fe/Fe_3O_4 nanoparticles, confirming that the complex nanoparticles with core/shell morphology can optimise the heating properties for hyperthermia. We also investigate the effect of interparticle interactions on the magnetic properties of assemblies of core/shell nanoparticles using a mesoscopic model of a few spins [3] that describes efficiently the complex structure of each nanoparticle. The dipole-dipole interparticle interaction effects on the heating performance are presented for various concentrations. Our simulations show that the hyperthermia performance reduces for higher concentrations in the case of random assemblies. For NP arrays we have increase of this performance with the concentration.

1. C Binns et al. J Nanopart Res (2012) 14:1136
2. M. Vasilakaki, C. Binns and K. N. Trohidou, Nanoscale, 7, 7753-7762 (2015)
3. G. Margaris, K. N. Trohidou, J. Nogués, Adv. Mat. 24 4331 (2012)