Cube Model Approach in Simulating of Magnetite Nanoparticles Behaviour in External Magnetic Fields

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Abstract. *Iron 'overloading' can lead to various health complications, such as diabetes, cirrhosis, and heart disease. Moreover, biogenic iron oxides nanoparticles, found in human brain tissue are connected to neurodegenerative processes. MRI represents potential tool in non-invasive body-iron quantification, because iron strongly affects the MRI signal. However, iron oxides nanoparticles are with respect to behaviour in external magnetic fields, generally approximate to a 'Sphere' model. This can lead to incorrect evaluation. Here, we introduce a more realistic 'Cube' model, with two approaches: (i) cell unit (CU), and (ii) bulk, with almost identical results.*

Keywords: Magnetite Nanoparticles, Cube Model, MRI, Body-Iron Evaluation

1. Introduction

Recently, biogenic iron oxides (magnetite) nanoparticles have been found in several animal species, including humans [1]. Biological magnetite is produced by genetically-controlled biochemical process, and in animal species plays a crucial role in geomagnetic navigation [2]. Its role in humans is still unclear, but elevated levels of magnetite particles are associated with neurodegenerative disorders [3]. However, an "iron overloading" can lead to various other complications, such as diabetes, cirrhosis, and heart disease [4]. Therefore, the proper quantification method of body-iron is crucial in diagnostics. Iron strongly affects relaxation times of protons during MRI and causes such a contrast enhancement of examined tissue. It predestines the MRI to become a completely non-invasive body-iron diagnostic method. Because body-iron is usually in a form of iron oxides, we have chosen magnetite nanoparticles as a model system. However, magnetite nanoparticles are in external magnetic fields generally approximated to a sphere with radius ≈ 10^{-7} m and magnetic moment ≈ $2\text{x}10^{-15}$ Am^2 [5]. Here, we introduce practically more intuitive and accurate 'Cube' model method with two approaches: (i) cell unit (CU), and (ii) bulk.

2. Subject and Methods

Sphere model approximation represents magnetite nanoparticles as the sphere with radius ≈ 10^{-7} m and magnetic moment ≈ $2\text{x}10^{-15}$ Am^2. We introduce 'Cube' model method with two approaches: (i) cell unit (CU), and (ii) bulk. Because of biological origin of biogenic magnetite nanoparticles, we take into consideration only single-domain particles with (cube) dimension a_{mag} = 4 – 500 nm [6].

In '*CU' approach*, a magnetic moment of particle is derived from cell unit (CU) shape and size of the particle. Magnetite CU is made from 8 formula units (FU) and belongs to isometric – hexoctahedral crystal system (space group Fd3m) with cell dimensions $a_{CU} = 0.83958\ nm$ and volume $V_{CU} = 5.9182x10^{-28}\ m$. Magnetic moment for particle was calculated as follows:

$$\vec{\mu}_{mag(CU)} = N_{CU}\vec{\mu}_{CU} = \frac{V_{mag}}{V_{CU}} 8\vec{\mu}_{FU} = 34.64\frac{V_{mag}}{V_{CU}}\mu_B \qquad (1)$$

where N_{CU} is the number of CU in particle and $\mu_{FU} = 4.33\ \mu_B$ [7], where μ_B is the Bohr magneton.

In *'Bulk' approach*, the magnetic moment is derived from equation

$$\vec{\mu}_{mag(Bulk)} = M_{sat(Bulk)} m_{mag} = M_{sat(Bulk)} \frac{V_{mag}}{V_{CU}} m_{CU} = M_{sat(Bulk)} \frac{8a^3 Mr(Fe_3O_4) m_u}{V_{CU}} \quad (2)$$

where $M_{sat(Bulk)}$ is the saturation magnetization (for magnetite $M_{sat(Bulk)} \approx 90\ Am^{-2}kg^{-1}$), m_{mag} is the mass of one magnetite nanoparticle with cube dimension a, M_r is a molecular weight of magnetite, and m_u is an atomic mass constant.

We determined nanoparticle magnetization $\mathbf{M}_{mag}$ (which is size and temperature dependent) in magnetic field $\mathbf{B}$ applying Langevin function:

$$\vec{M}_{mag}(a,T) = M_{sat} m_{mag} [\coth(x) - 1/x] \quad (3)$$

where m_{mag} is the mass of magnetite particle and $x = \mu_{mag}B/k_BT$. The values of saturation magnetization M_{sat} for magnetite nanoparticles were determined experimentally (for $a = 4; 11.5; 47.7; 150\ nm \rightarrow M_{sat} = 31.8; 60.1; 65.4; 75.6\ Am^2kg^{-1}$ at $T = 300\ K$ [8]).

3. Results and discussion

In **Figure 1** is shown comparison of models for nanoparticles magnetic moment calculation. Cube models approaches represent our proposed method and sphere model represents general approximation. Stability of information, saved in preservation of particle's magnetic moment direction is shown in **Figure 2**.

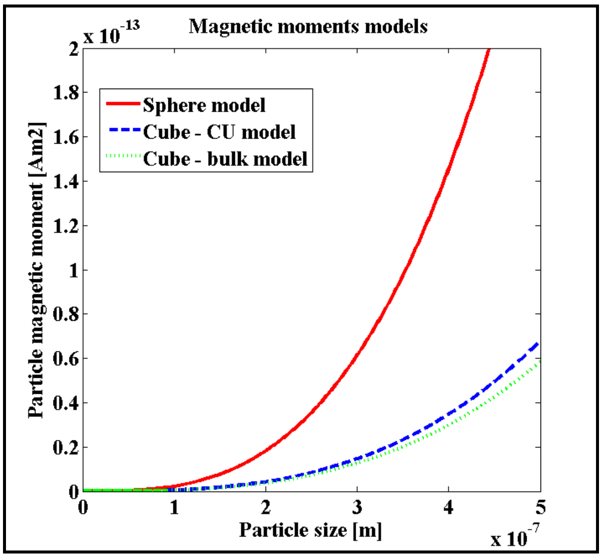

Fig. 1. Comparison of magnetic moment values in magnetite nanoparticles, for generally used 'Sphere' model and our proposed 'Cube' model with cell unit (CU) and bulk approaches. Magnetic moments for "Sphere model are calculated in the same manner than for "Cube model", but with a_{mag} as a radius.

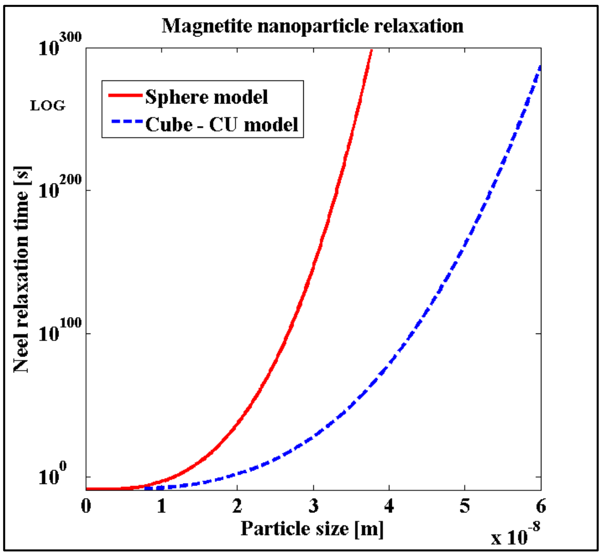

Fig. 2. Néel relaxation times for magnetite nanoparticles depending on size of particles ($\tau_0 \approx 10^{-9}$s, K=13.5 kJm^{-3}). Y axis is in LOG scale. It is evident that magnetite nanoparticles are suitable as information storage medium. We compare our 'Cube model' approach and "Sphere model' approach.

Magnetization of magnetite nanoparticles for different sizes, and in strong magnetic fields, is shown in **Figure 3a-d**. It is obvious, that for high magnetic fields the differences between models are insignificant. However, for low magnetic fields the differences are important and using an incorrect model can lead to wrong conclusions. This is demonstrated in **Figure 4**, where is shown Geomagnetic-field rotational work dependence on size of particle. Magnetic field of the Earth varies form ≈ 30 μT to ≈ 60 μT (for our latitude ≈ 50 μT).

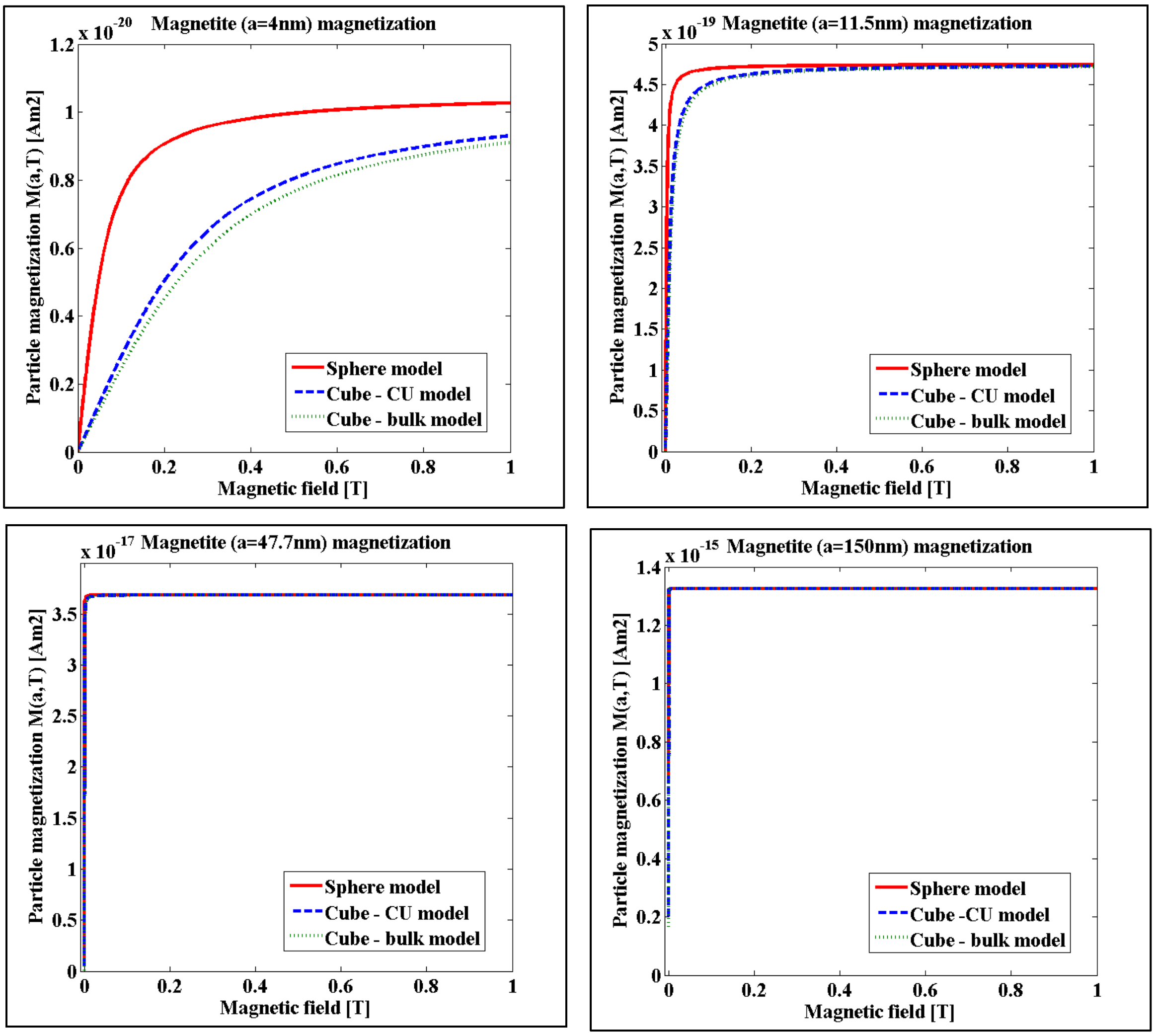

Fig. 3. Comparison of magnetite nanoparticles magnetization values for generally used 'Sphere' model and our proposed 'Cube' model with cell unit (CU) and bulk approaches, in magnetite nanoparticles with different sizes: (a) 4 nm, (b) 11.5 nm, (c) 47.7 nm, and (d) 150 nm.

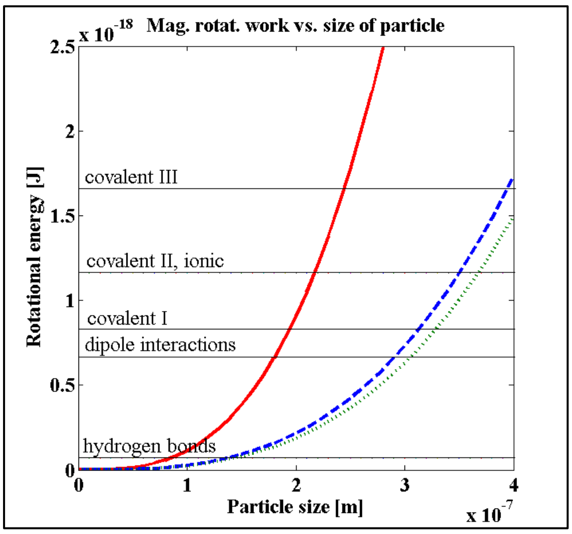

Fig. 4. Magnetic rotational work vs. size of magnetite nanoparticle (for range 0 – 400 nm) in magnetic field of the Earth. Comparison of 'Sphere' model and our 'Cube' model with cell unit and bulk approach. Horizontal lines represent maximum level in typical biochemical bond energy. As seen, energies associated with rotational work of geomagnetic field on the magnetite nanoparticles correlate with energies of biochemical interactions. Calculated for $\theta = \pi/2$.

4. Conclusions

We showed, that for strong magnetic field (>1T) and larger particles (>50nm), the magnetization of magnetite nanoparticles is almost identical for 'Sphere' and 'Cube' model approach. However, for smaller particles (ferritin-like), the differences are quite distinct, and the use of incorrect model can lead to incorrect MRI body-iron evaluation. There are also big differences between models in determination of magnetic moments for particles bigger than 100 nm. Cube model represents more realistic approach and apart from body-iron evaluation can be helpful in determination of contrast agent efficiency, evaluation of electromagnetic hazard, or other issues related to iron oxides nanoparticles.

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