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Energy distribution in iron nano-spheres with cubic magneto-crystalline anisotropy

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Introduction & Aim

- Magnetic memory systems are recently strongly investigated in the research area of spintronics. Amongst the different data storage systems, magnetic nanoparticles are of high interest since they can often store large amounts of data on small scales [1].
- Such magnetic nanoparticles, however, pose new challenges, such as oxidation and agglomeration [2].
- Here we show micromagnetic simulations using MagPar [3], solving the Landau-Lifshitz-Gilbert (LLG) equation using finite elements, to analyze the energy density of iron nano-spheres with and without oxide shell. For spheres of 10 nm or 25 nm radii and different oxide shell thicknesses, 3D energy maps are calculated [4].

Materials and Methods

- *r* = 10 nm: shell thickness = 0 nm … 9.8 nm, 0.2 nm steps
- *r* = 25 nm: shell thickness = 0 nm … 24.5 nm, 0.5 nm steps
- Initial simulation state: uniform, single-domain
- Calculate deflection angle between initial (i) and final (f) orientation: $\alpha = \sphericalangle\left(\vec{M}_i^{(s)}, \vec{M}_f^{(s)}\right)$ for single (s) droplet and $\alpha = max\sphericalangle\left(\vec{M}_i^{(m)}, \vec{M}_f^{(m)}\right)$ for multiple-droplet (m) system

→ Let system relax into nearest energy minima, starting from diverse orientations of the magnetization, to map energy

Anisotropies taken into account for Fe nano-droplets:

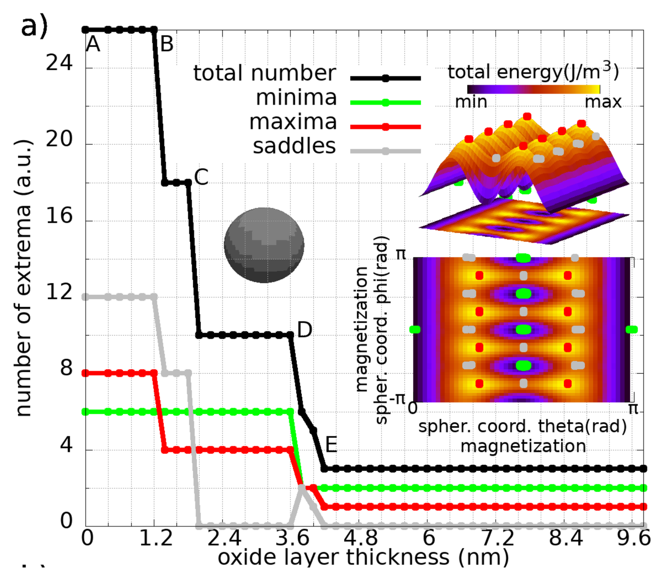
- magneto-crystalline cubic anisotropy with axes along the polar angle θ = 0 (out-of-plane) and φ = 0 (in-plane), and constants $K_1 = 4.8{\cdot}10^4$ J/m³ and $K_2 = 5.0{\cdot}10^3$ J/m³
- exchange constant $A = 2{\cdot}10^{-11}$ J/m
- magnetic polarization at saturation $J_s = 2.1$ T

For oxidized shell layers (γ-Fe_2O_3, maghemite):

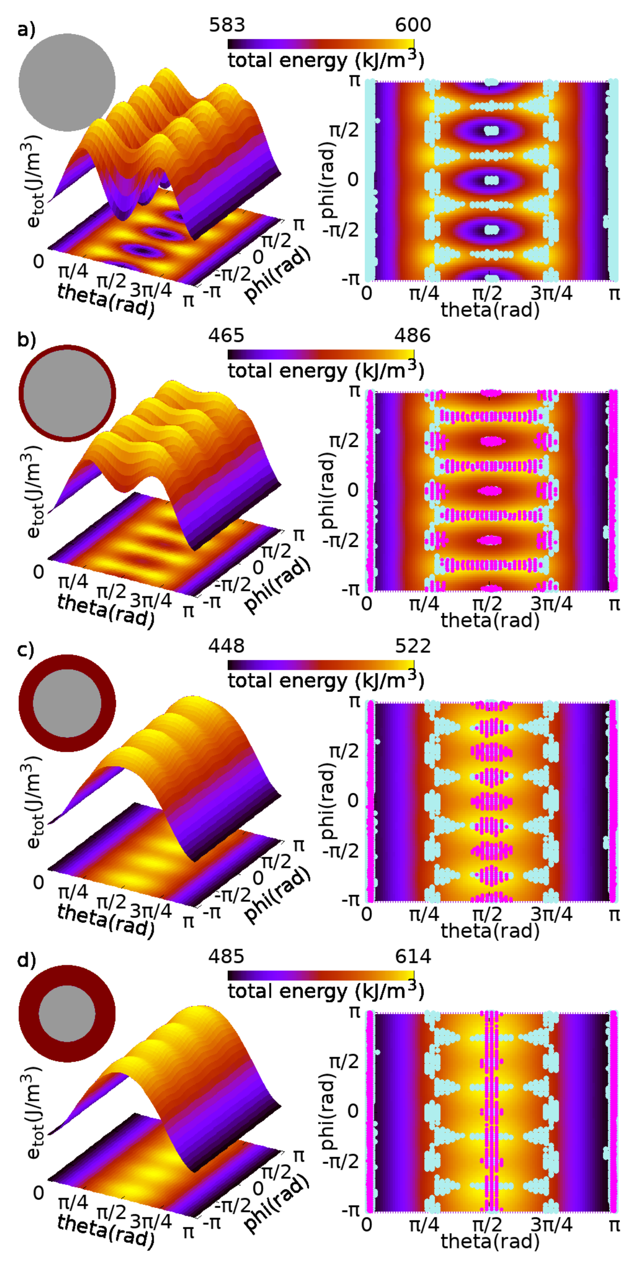
- uniaxial anisotropy constant $K_1 = 4.0{\cdot}10^4$ J/m³
- exchange constant $A = 1.32{\cdot}10^{-11}$ J/m
- magnetic polarization at saturation $J_s = 0.4$ T

Results

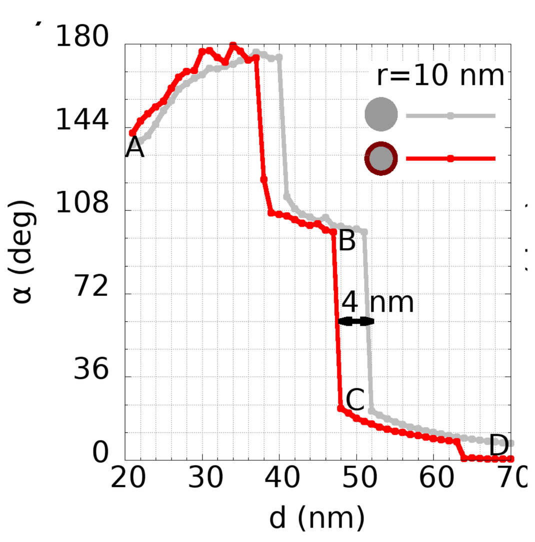
Numbers of energy extrema as a function of oxide layer thickness for the 10 nm sphere radius.
Inset: 3D map of total energy with color-coded extrema and 2D map of total energy with color-coded reference points placed in energetic extrema



Results of the *r* = 10 nm droplet with oxide layer thickness equal to (**a**) 0 nm, (**b**) 1.2 nm, (**c**) 3.4 nm, and (**d**) 4.2 nm, respectively.
Light-blue dots indicate convergence orientations (of all possible types) for the 0 nm layer case (a). They are also placed in sub-figures (b), (c), and (d) to compare the convergence ability of the oxidized samples with the convergence orientations of the un-oxidized sample – the final convergence positions of the oxidized spheres are marked here by violet dots. The circles in the upper left corners of each picture are sketches of the respective droplets.



Comparison of 10 nm four-sphere systems, showing deviation angle α as function of d (distance between sphere centers). The red graph shows the influence of a 1 nm oxide layer, decreasing the distortion level at short distances, supporting high writing-density memor



Literature

[1] Simeonidis, K.; Martinez-Boubeta, C.; Serantes, D.; Ruta, S.; Chubykalo-Fesenko, O.; Chantrell, R.; Oró-Solé, J.; Balcells, L.; Kamzin, A. S.; Nazipov, R. A.; Makridis, A.; Angelakeris, M. Controlling Magnetization Reversal and Hyperthermia Efficiency in Core−Shell Iron−Iron Oxide Magnetic Nanoparticles by Tuning the Interphase Coupling, *ACS Appl. Nano Mater.* **2020**, *3*, 4465.
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Conclusion

- The cubic magneto-crystalline anisotropy leads to a non-uniform energy distribution of the magnetic nano-spheres, with the number of extrema decreasing for larger oxide layer thicknesses.
- In case of agglomeration of four nano-spheres, the distances between the nano-spheres strongly modify the system's magnetic properties, where an oxide shell enables bringing the nano-spheres closer together before they start influencing each other, as seen by comparing the magnetic properties of these agglomerates with the single nano-spheres.
- For the oxide coated system, the maximum packing density could be increased by about 12%, as compared to the non-coated system, indicating that a higher data density can be reached by preparing a matrix of magnetic nano-spheres with oxide shells.

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