Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Elucidating the role of shape anisotropy in faceted magnetic nanoparticles using biogenic magnetosomes as a model

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FEM Model

To solve an electromagnetic problem on a macroscopic level we use Maxwell's equations subjected to certain boundary conditions. Usually, it is helpful to formulate the problem in terms of the electric scalar potential Φ, and the magnetic vector potential $\vec{A}$. In our case, there are no currents present, so the equations of interest for us are:

$$\vec{B} = \nabla \times \vec{A} \quad (1)$$

$$\nabla \times \vec{H} = 0 \quad (2)$$

We solve the model using these expressions together with the constitutive relation:

$$\vec{B} = \mu_0(\vec{H} + \vec{M}) \quad (3)$$

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The magnetization is kept constant along an arbitrary direction given by unit vector $\hat{u}_m$, $\vec{M} = M\hat{u}_m$, where the magnetization module is set as the saturation magnetization of magnetite, *M* = 480 kAm^{-1}. Moreover, the 3D model is formed by the desired figure enclosed within air, to choose, in this way, suitable boundary conditions (**Figure S1**a-b). At the ends of the air domain, we imposed magnetic insulation:

$$\vec{n}\, x\, \vec{A} = 0 \quad (4)$$

Taking all this into account, we can calculate for a desired figure, the $\vec{B}$ and $\vec{H}$ field within the particle at all points (Figure S1c-d). We do this fixing the magnetization as a constant in the entire solid angle of the particle, and evaluating for all the cases the total magnetostatic density energy of the particle (Figure S1e):

$$E_{magn} = \oint -\frac{1}{2}\mu_0 \vec{H}_d \cdot \vec{M} dV \qquad (5)$$

Given that magnetic poles distribution depends on where the magnetization points to, magnetostatic energy given by Equation (5) is angle-dependent and therefore encloses a form of magnetic anisotropy called shape anisotropy.

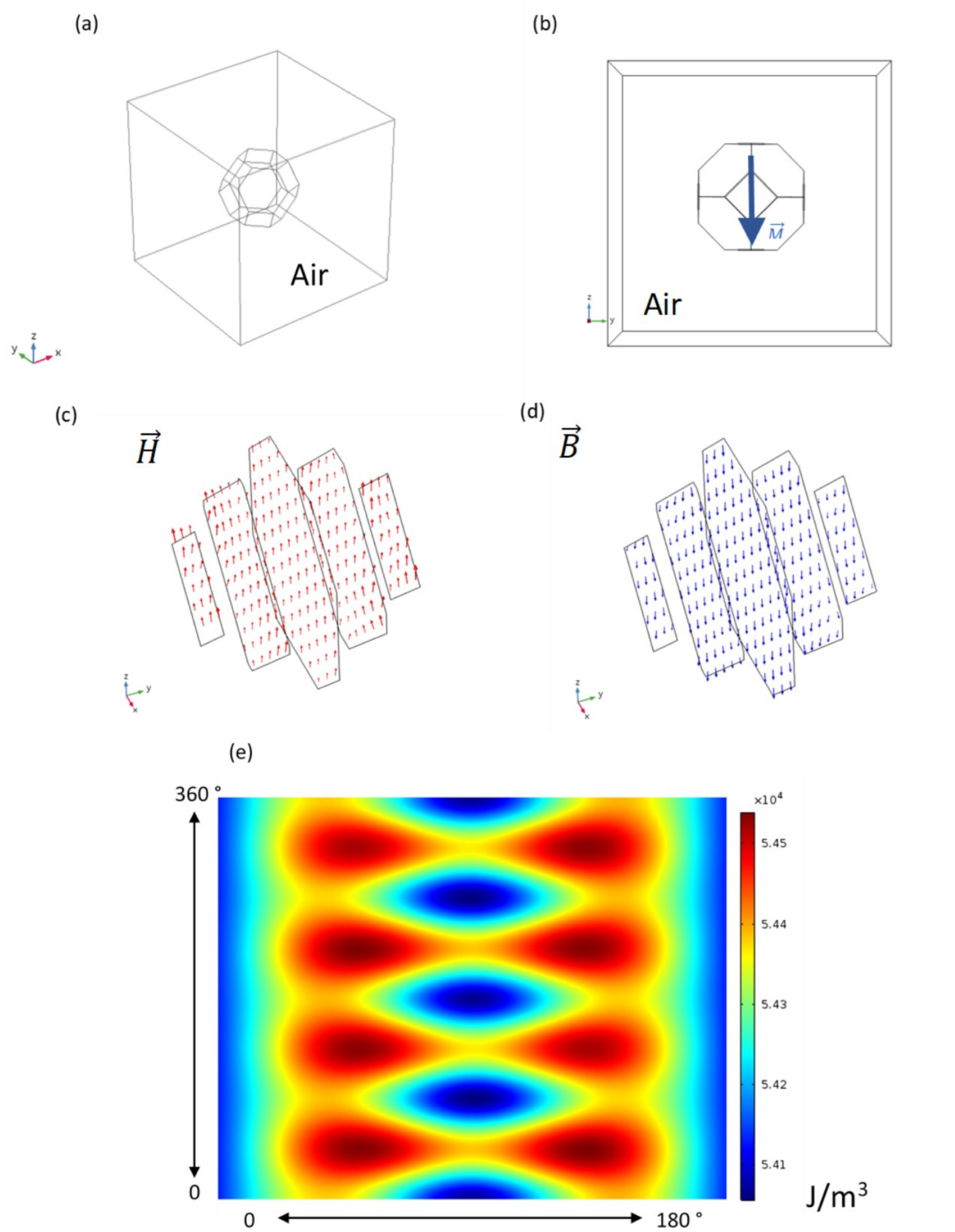

Figure S1. (a) Perfect truncated octahedron surrounded by air domain. (b) XZ slice of the Truncated octahedron . (c) $\vec{H}$ field of several XZ slices of the truncated octahedron. (d) $\vec{B}$ field of several XZ slices of the truncated octahedron. (e) 2D vision of the positive cubic shape anisotropy of the truncated octahedron.