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Supplementary information
Configuration of the magnetosome chain: a natural 1D magnetic nanostructure

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TEM image of oriented bacteria

Fig. 1 shows a TEM image of aligned *Magnetospirillum gryphiswaldense* cells deposited onto a Si substrate under an aligning field H_{al}.

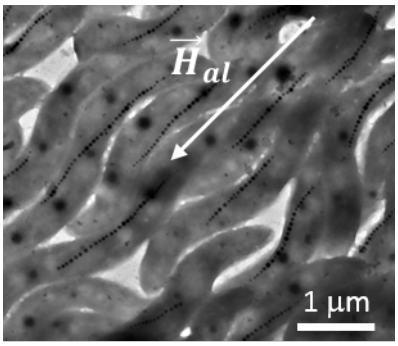

Figure 1: TEM image of bacteria arranged in a 2D configuration with their chain axes oriented along the aligning field (H_{al}).

Calculation of the hysteresis loops

Magnetosomes along the chain have been managed as a collection of independent single domain particles which are large enough to be thermally stable and so to have the magnetization firmly anchored at the minimum energy states. Inter-particle dipolar interactions are assumed to impose an additional anisotropy contribution, equal for all, referred to as 'interaction' anisotropy. The functional form of the energy density for a magnetic single domain depends on the orientation of magnetization given by two variables (polar and azimuthal angles in spherical coordinates). Such energy density landscape $E(\theta, \varphi)$, in the presence of arbitrary external magnetic fields contains the magnetic anisotropy terms (that includes dipolar interactions) plus the Zeeman energy:

$$E(\theta, \varphi) = E_{anisotropy}(\theta, \varphi) + E_{Zeeman}(\theta, \varphi) \tag{1}$$

For a given function $E(\theta, \varphi)$, determination of M_H (magnetization projection over $\vec{H}$) is performed by a simple dynamical approach in which the single domain magnetization can switch between the available energy minima states at a rate determined by a Boltzmann factor[1,2]. This factor depends on the energy barriers ($E_b V$, where V is the particle volume) between such minima ($\sim \exp(-E_b V/k_B T)$) and can be calculated from the field dependent energy landscape.

For the calculation, the magnetization is given by:

$$M_H(\vec{H}) = M \sum_i p_i(\vec{H}) \hat{u}_i(\vec{H}) \cdot \hat{u}_H \tag{2}$$

where $p_i(\vec{H})$ are the probabilities of finding the magnetization at state i ($i = 1$ or 2), $\hat{u}_i(\vec{H})$ are the director vectors of energy minima, dependent on the external field $\vec{H} = H\hat{u}_H$. The quasi-static condition for the externally applied magnetic field in DC magnetometry can be reproduced by a slowly varying sinusoidal field ($H(t) = H_0 \sin \omega t \hat{u}_H$), of frequency much smaller ($\sim 1\,\mathrm{Hz}$) than the natural frequency of jumps attempts of electron spins ($10^9\,\mathrm{Hz}$), of the order of the

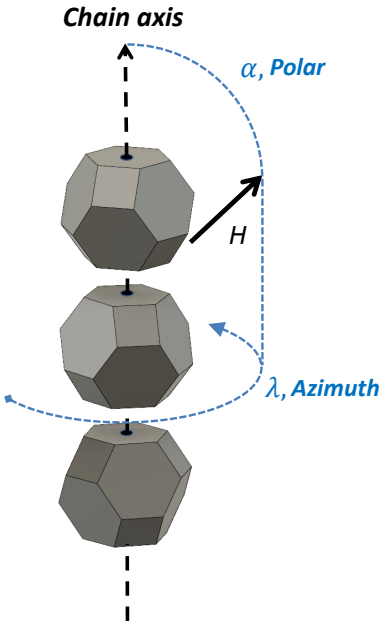

Figure 2: Polar (α) and azimuthal (λ) angles defining the orientation of the external field relative to the chain axis.

Larmor precession frequency, denoted by $\nu_0 \sim 10^9$ Hz. The latter determines the rate of jumps between minima which is dependent on the applied field, given by $w_{ij} = \nu_0 \exp(-VE_{ij}/k_BT)$, where E_{ij} is the energy density barrier between minima i and j. The barriers E_{ij} are calculated from the particular energy density landscape $E(\theta, \varphi)$.

In this way, probabilities $p_i(\vec{H})$ become time-dependent functions $p_i(t)$ that can be calculated by numerically solving ordinary differential equations as:

$$\frac{\partial p_i}{\partial t} = \sum_{j \neq i} w_{ji} p_j - \Big(\sum_{j \neq i} w_{ij} \Big) p_i \tag{3}$$

This continuity equation reflects the simple fact that the increment of population i results from the balance between incoming jumps (first term) and outcoming jumps (second term) to or from the rest of the minimum states, with the conservation of magnetization condition given by $\sum p_i = 1$.

Either because the whole chain is free to rotate around itself or because magnetosomes can

be rotated relative to each other, simulations for the whole chain for a given orientation between the external field H and the chain axis (angle α, in the scheme of Fig. 2) must be averaged for the equally probable azimuthal orientations (between 0° and 360°) relative to the polar axis defined by the chain:

$$M(H) = \int_0^\pi M_H(H, \lambda) d\lambda \tag{4}$$

where $M_H(H, \lambda)$ is the magnetization as a function of external field for a given orientation of the azimuthal angle λ, which exact definition will depend on the particular reference system of the problem.

Except for the case of external field applied parallel to the chain ($\alpha = 0$), where all particles are equivalent by symmetry, the resultant hysteresis loop is calculated by averaging 18 single loops from $\lambda = 0^\circ$ to $\lambda = 180^\circ$ in steps of 10°. In the random case (un-oriented bacteria), simulation is obtained by averaging simulations for all the orientations weighted by $\sin \alpha$. In this way, the simulation needs the calculation of 180 single simulations.

Calculation of the chain energy

The total energy of the chain has been estimated as the sum of the magnetostatic interactions between nanoparticles and the contribution of the lipid/protein-based architecture embedding the magnetosome chain.

The magnetostatic interactions are straightforward to implement in the point dipole approximation: the dipolar magnetic energy is the sum of all dipole pair potential energies between particles, where particles are taken as uniformly magnetized spheres:

$$U_m = \frac{1}{2}\frac{\mu_0 m^2}{4\pi}\sum_{i,j}^{N}\frac{1}{r_{ij}^3}[\hat{u}_i \cdot \hat{u}_j - 3(\hat{u}_i \cdot \hat{u}_{ij})(\hat{u}_j \cdot \hat{u}_{ij})] \tag{5}$$

where N is the total number of particles in the chain, $\hat{u}_i$ is the dipole unit vector of particle i, $\vec{r_{ij}} = r_{ij}\hat{u}_{ij}$ is the vector position of particle j from particle i. $m = M_s V$ is the magnetic moment of particles, where $V = \pi D^3/6$ is the volume and D the particle diameter. The magnetic moments m are assumed identical for simplicity, and according to the proposed anisotropy model they form a fixed polar angle of 20° with respect to the chain axis.

The contribution to the total chain energy from the lipid/protein-based architecture inside bacteria is much more challenging to quantify. For the sake of simplicity we follow two assumptions. Firstly, we consider that the inter-particle distance is constant ($r_{i,i+1} \equiv d$). This means that chains can bend or twist but cannot stretch. Secondly, the forces exerted on each particle work like springs acting perpendicularly to the z axis and proportional to the projection on the horizontal plane of the relative vector positions. In this way, the spring-like elastic energy can be expressed as:

$$U_{elastic} = \frac{1}{2}kd^2\sum_{i}^{N}[2 - (\hat{u}_{i,i+1} \cdot \hat{u}_z)^2 - (\hat{u}_{i,i-1} \cdot \hat{u}_z)^2] \tag{6}$$

Here, d is the center-to-center inter-particle distance and k is the elastic constant. Except for particles at both ends, each particle is subjected to forces from two nearest neighbors ($i+1$ and

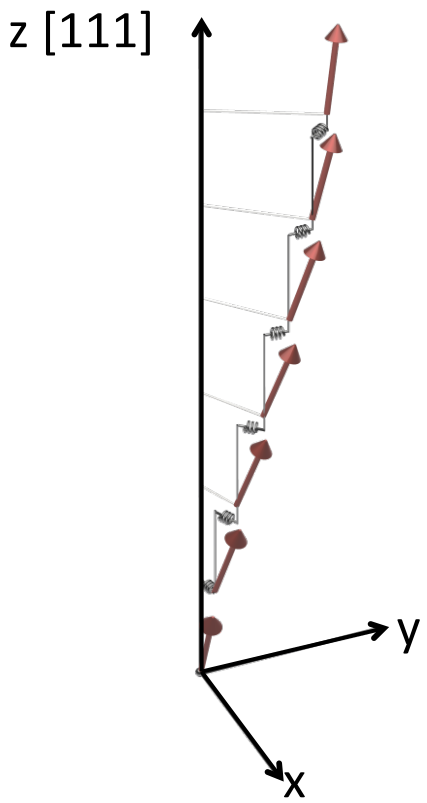

Figure 3: Sketch showing the orientation of the magnetic dipoles and the elastic force acting on them.

$i-1$), as expressed by the terms inside the summation in eq. 6. Fig. 3 sketches the orientation of the magnetic dipoles together with the elastic force acting on them.

The total chain energy is then $U = U_m + U_{elastic}$, and only three independent variables per particle are enough to determine the energy of the chain, namely the radial (ρ) and azimuthal (ϕ) coordinates for the positions, and azimuthal orientation (φ) of the magnetic dipoles.

Stable configurations of the chain can then be calculated by minimizing the total energy U.

2D projection of the magnetic dipoles

Fig. 4 right shows the 2D projection on the yz plane of the magnetic dipoles of the chain section shown on the left, aimed to highlight that in a 2D projection such as those from electron holography imaging[3], apparent tilting between consecutive dipoles is no more than 7°.

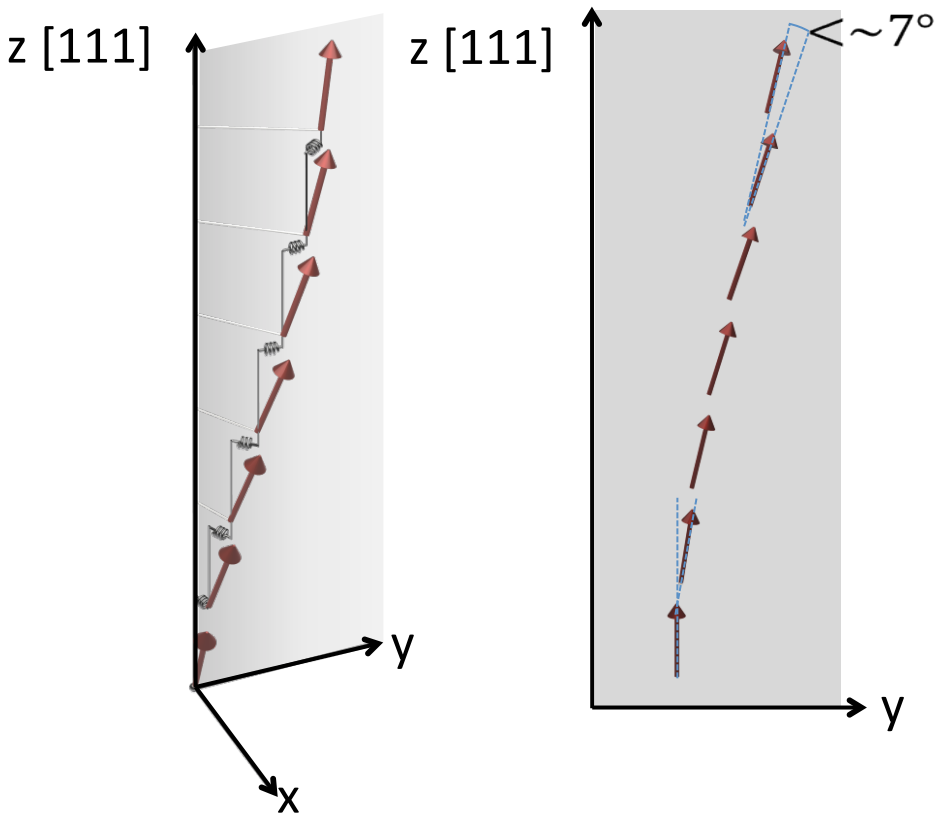

Figure 4: 2D projection of the magnetic dipoles in the chain section shown on the left.

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