Supporting information

Effect of albumin coating on the magnetic behavior of Mn ferrite nanoclusters

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Short description of the mesoscopic model and the parameters

The mesoscopic model that simulates an assembly of Mn ferrite nanoparticles of diameter *D* = 2 nm with a core/surface morphology and the exchange inter-particle and long range dipolar interactions it has been described in ref [1] and for an albumin coated assembly in ref [2]. The energy of the system is given by the following expression [3]:

$$
\begin{aligned}
E = & -\sum_{i=1}^{N} K_c V_1 \left(\vec{s}_{1i}\cdot\hat{e}_{1i}\right)^2 - \sum_{i=1}^{N} K_{srf}\left[V_2\left(\vec{s}_{2i}\cdot\hat{e}_{2i}\right)^2 + V_3\left(\vec{s}_{3i}\cdot\hat{e}_{3i}\right)^2\right] \\
& -\frac{1}{2}\sum_{i=1}^{N}\left[J_{c1}\left(\vec{s}_{1i}\cdot\vec{s}_{2i}\right) + J_{c2}\left(\vec{s}_{1i}\cdot\vec{s}_{3i}\right) + J_{srf}\left(\vec{s}_{2i}\cdot\vec{s}_{3i}\right)\right] \\
& -\frac{1}{2}g\sum_{i,j=1,i\neq j}^{N}\left(m_{1i}\vec{s}_{1i} + m_{2i}\vec{s}_{2i} + m_{3i}\vec{s}_{3i}\right)D_{ij}\left(m_{1j}\vec{s}_{1j} + m_{2j}\vec{s}_{2j} + m_{3j}\vec{s}_{3j}\right) \\
& -\frac{1}{2}J_{intra\text{-}cluster}\sum_{<i,j>}\left[\left(\vec{s}_{2i}\cdot\vec{s}_{3j}\right) + \left(\vec{s}_{3i}\cdot\vec{s}_{2j}\right)\right] - \mu_0 H\sum_{i=1}^{N}\left(m_{1i}\vec{s}_{1i} + m_{2i}\vec{s}_{2i} + m_{3i}\vec{s}_{3i}\right)\cdot\hat{e}_h
\end{aligned}
\qquad \text{(S1)}
$$

Here each Mn nanoparticle is described with a classical spin ($\mathbf{s}_{1i}$) for the core and two spins ($\mathbf{s}_{2i}$, $\mathbf{s}_{3i}$) for the two surface sublattices. We have calculated the normalized magnetic moments $m_1 = M_1V_1/M_sV$ $m_2=M_2V_2/M_sV$ and $m_3=M_3V_3/M_sV$, where M_s and V are the saturation magnetization and the volume of each particle and V_1,V_2,V_3 and M_1,M_2,M_3 are the particle volumes and magnetizations of the core spins and the two sublattices of the surface spins respectively. From atomic scale calculations described in ref [1] these parameters are m_1=0.1, m_2=0.5, m_3=0.4. Since DFT calculations indicate that the surface magnetic moments

are reduced due to the existence of albumin, we consider m_2 =0.45 and m_3=0.4 for the coated nanoparticles. D_{ij} is the dipolar tensor and $g = \mu_0(M_sV)^2/(4\pi d^3\ 20K_CV_1)$ is the reduced dipolar strength we set g = 3.0.

The effective anisotropies for the core is taken k_c=0.05 and for the uncoated surface k_{srf} =1.0 for each spin calculated in detail in reference [1]. Since for the albumin coated sample, our DFT calculations indicate that the surface anisotropy is reduced due to the existence of the albumin [2], we set k_{srf}= 0.8.

The effective intra-particle exchange coupling constants are defined as j_{c1} ($\mathbf{s}_{1i}/\mathbf{s}_{2i}$), j_{c2} ($\mathbf{s}_{1i}/\mathbf{s}_{3i}$) and j_{srf} ($\mathbf{s}_{2i}/\mathbf{s}_{3i}$). In the uncoated particles j_{c1}= 0.5, j_{c2} = 0.45, j_{srf} = -1.0 and in the coated ones j_{c1} = 0.5, j_{c2} = 0.45, j_{srf} = -0.8 [2]. The j_{srf} is considered to be reduced owing to the metal-albumin bonding that causes the expansion of the neighboring magnetic atoms at the surface of the Mn ferrite nanoparticles, as indicated by our DFT calculations [2]. We consider that the albumin molecules cover a number of nanoparticles and create clusters, thus increasing the fraction of the shell that is in physical contact with the neighboring shells. Therefore, we take the inter-particle exchange coupling constant between the nanoparticles in each isolated cluster as $j_{intra\text{-}cluster}$ = -0.80, increased 60% from the inter-particle exchange coupling strength in the uncoated nanoparticle assembly (j_{inter}= -0.50) [1].

REFERENCES

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