Response of a Magnetic Nanoparticle System to a Rotating Magnetic Field

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The Model and Simulations: Stoner-Wolhfarth Model+Dipolar Interactions

Energy of the i^{th} Magnetic Nanoparticle (MNP) (reduced units):

$$e_i = -\frac{1}{2}(\hat{k}\cdot\hat{\mu}_i)^2 + \vec{h}\cdot\hat{\mu}_i + \vec{h}_d^{\,i}\cdot\hat{\mu}_i, \quad \text{with } \vec{h}_d^{\,i} = g\sum_{i\neq j}^{N_p}[\hat{\mu}_j - 3(\hat{\mu}_j\cdot\hat{r}_{ij})\hat{r}_{ij}]/r_{ij}'^3$$

Anisotropic energy — *Zeeman energy* — *Dipolar interactions energy*

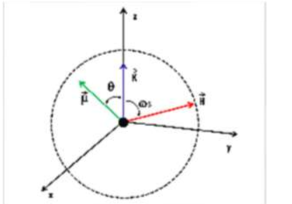
$$\vec{h} = \frac{\vec{H}}{H_A} = \frac{\mu_0 M_S \vec{H}}{2K},\ g = \frac{M_S}{H_A},\ r_{ij}' = \frac{r_{ij}}{D} \quad \text{so } t = \frac{k_B T}{2KV}$$

$\hat{\mu}_i$: Unit vector of the magnetic moment $\vec{\mu} = M_S V\hat{\mu}_i$;
M_S: Saturation magnetization, V: volume, D: diameter;
$\hat{k}$: Unit vector of the anisotropy axis $\vec{K} = K\hat{k}$ assumed uniaxial;
$\hat{r}_{ij}$: Unit vector that joins i and j MNPs,
g= Dipolar Interaction magnitude

Rotating External Magnetic Field:

$$\vec{h} = h_0(0, cos(\omega s), sin(\omega s))$$

ω=angular frequency, s= MCS time



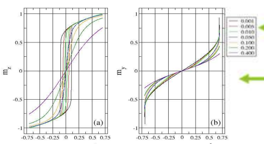
MNP Parameters and simulation Details

- *Fe MNP monodisperse Np =100 spherical particles with diameter D =7,5 nm, K=4,5 x 10^4, M_s=1,7 x 10^6 A/m;*
- *Néel relaxation is only allowed;*
- *The MNP´s were randonly distributed in a cubic box of size L=8 D;*
- *Direction of $\hat{k}$: along z axis, and random;*
- *Metropolis Dynamics with solid angle restriction* [Nowak]
- *Thermal reservoir at temperature t, open boundary conditions:*
- *The components of the normalized magnetization were measured every tm=120 MCS*

Results and Discussion:

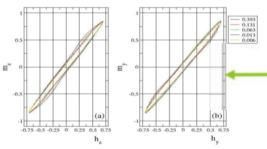
Non Interacting Model (Stoner-Wohlfarth-SW): g=0 [Stoner]

Frequency behavior with h_0=0.7 and t=10^{-4}: Hysteresis only in m_z for fixed $\hat{k}$ and in both components with $\hat{k}$ random



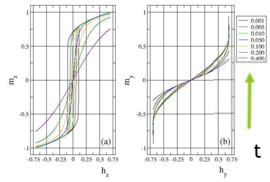
ω

Fixed $\hat{k}$

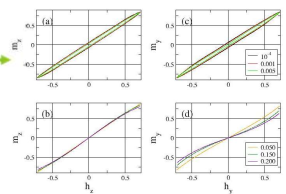


Random $\hat{k}$

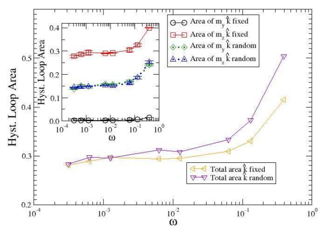
Thermal behavior with h_0=0.7, ω=0.006: vanishing of the blocked state



t

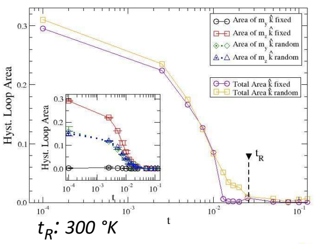


Hysteresis Loop Areas



In both cases, better heat transfers when the MNP´s anisotropy axes are directed randomly (no special preparation is required)

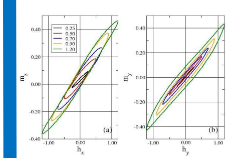
Hysteresis Loop Areas



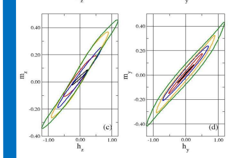
t_R: 300 °K

Interacting Model (Stoner-Wohlfarth+Dipolar interactions-SWD): g=1.6875

Low t Behavior: t=10^{-4}, ω=0.006: Rounded hysteresis loops that extend beyond the theoretical h_0 interval 0.5≤ h_0≤ 1.0 [Usov] *Displaced loops w/respect to the origin*

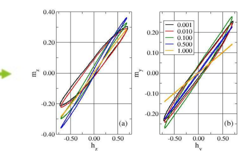


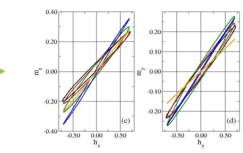
Fixed $\hat{k}$



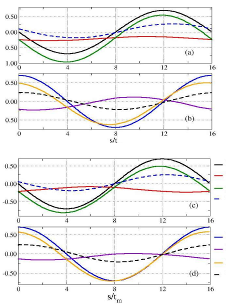
Random $\hat{k}$

Thermal Behavior: h_0=0.7, ω=0.006: Hysteresis in both components beyond t_R, displaced loops that center with t





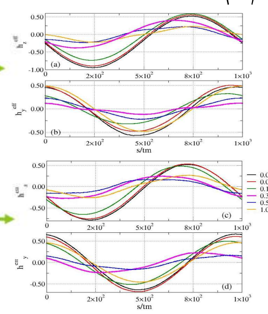
Dipolar field per particle: $\langle\vec{h_d}\rangle = {}^1/_{N_p}\sum_{i=1}^{N_p}\vec{h}_d^{\,i}$,



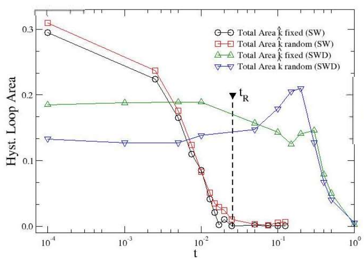
Fixed $\hat{k}$ — Random $\hat{k}$

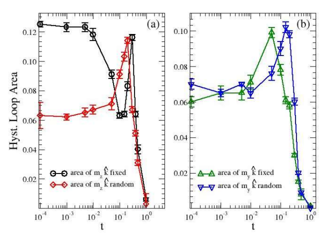
At this temperature, the dipolar field affects the action of the external field causing an effective field that is not symmetrical with respect to the zero-field line, So the values of the coercive field in both components are not symmetric. This effect is less relevant in the y components

Effective field: $\vec{h}^{eff} = \vec{h} + \langle\vec{h_d}\rangle$:



For 10^{-3}≤ t≤ 0,5 the effective fields behave as in the t=10^{-4} case since the dipolar field components are negative, and the loops are displaced
For t>0.15 (not shown) h_z^{eff}(s)=h_z^{eff}(s±p/2) where $p = 1/\omega$, so the loops become more centered.





The peak exhibited in the areas is related to the termal activation of The dipolar field by temperature and the consequent apparition of the shape anisotropy in the blocked state [Saracco]

Conclusions:

SW model:

- The appearance of hysteresis with temperature in the magnetization components depend on the direction of the anisotropy axes;
- As a function of ω or t, the total area is larger for the random case, and increases the frequency.

SWD model:

- Hysteresis was observed for all coplanar magnetization components;
- The loop displacement is a consequence of the values of the dipolar field and the phase shift with the external field;
- The peak in the loop areas is associated with an anisotropy increase caused by the dipolar field.
- By comparing the total loop areas, the SW model can transfer an amount of heat than the SWD model at low temperatures, but this behavior is reversed for t≥ t_R

References:

[Stoner] E. C. Stoner and A. Wohlfarth, Trans R. Soc. Lond. A **240**, 826 (1948)
[Nowak]; U. Nowak, R. W. Chantrell and E. C. Kennedy,.Phys. Rev. Lett **84**(1):163-6, (2000)
[Usov] N. A. Usov, E. M. Gubanova, N. B. Epshtein, G. A. Belayeva, V. A. Oleinikov, J. Magn. Magn. Mater. **499**, 166260 (2020)
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