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Influence of the nanoparticle size on the blocking temperature of interacting systems: Monte Carlo simulations

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ABSTRACT

Zero field cooling curves (ZFC) under a relatively big magnetic field have been simulated in order to study the influence of the nanoparticle concentration on the rate of increase of the blocking temperature and its dependence with the nanoparticle size. Results show that for all nanoparticle concentrations the blocking temperature increases linearly with the nanoparticle size. The rate of increase of the blocking temperature is larger for larger nanoparticle concentrations, although it tends to a constant value for very large interactions between particles.

1. Introduction

Ensembles of single domain magnetic nanoparticles are very important in a wide range of applications. These systems display superparamagnetism at high temperature [1]. The superparamagnetic state occurs when the anisotropy energy of nanoparticles is overcome thermally. On lowering the temperature, the particles become blocked at a specific temperature, which represents the threshold of thermal activation.

According to the Stoner–Wohlfarth model the blocking temperature is given by [2]

$$T_B = \frac{KV}{\ln(\tau_m/\tau_o)k_B}, \tag{1}$$

where k_B is the Boltzmann constant, V is the particle volume, K is the anisotropy constant, τ_m is the measuring time and τ_o is a characteristic constant of particles that it is related to gyromagnetic precession.

The value of T_B can be modified by applying a magnetic field or changing the interactions between the magnetic nanoparticles.

Although the role of dipole–dipole interactions has been extensively studied [3–6], its effect is not clear and sometimes contradicting results were published. In order to clarify the role of these interactions, we have studied by Monte Carlo simulations of ZFC curves, the influence of the nanoparticle concentration on the rate of increase of the blocking temperature with the nanoparticle size when a moderate magnetic field is used.

2. Simulation model

A system of $N = 64$ monodisperse nanoparticles was placed in a cubic simulation cell where they have fixed positions with Lennard–Jones liquid-like arrangement [7–10]. The easy axes were chosen randomly.

The energy of the system is given by [7,8]

$$E = -\sum_i KV_i\left(\frac{\vec{\mu}_i\,\vec{n}}{|\vec{\mu}_i|}\right)^2 - \vec{\mu}_i\,\vec{H} + \sum_i\sum_{j\neq i}\frac{1}{2}\left(\frac{\vec{\mu}_i\,\vec{\mu}_j}{r_{ij}^3} - \frac{3\left(\vec{\mu}_i\,\vec{r}_{ij}\right)\left(\vec{\mu}_j\,\vec{r}_{ij}\right)}{r_{ij}^5}\right), \tag{2}$$

where $\vec{\mu}_i$ is the magnetic moment of the particle i, $\vec{n}_i$ is the unit vector in the easy direction, $\vec{r}_{ij}$ is the vector between particles i and j and $\vec{H}$ is the applied magnetic field.

For the superparamagnetic behavior it is assumed single domain magnetic particles with all its atomic magnetic moments rotating coherently. This results in a total magnetic moment given by $|\vec{\mu}_i| = M_S V$, where M_S is the saturation magnetization. M_S and K are assumed to be independent of the particle volume and the temperature of the system. The value of the applied field is $H = 0.4 \cdot H_o$, being $H_o \equiv 2K/M_S$ the anisotropy field.

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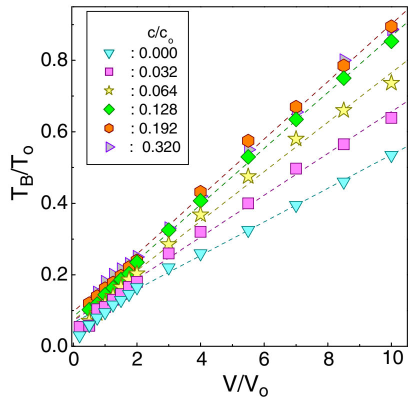

Fig. 1. Reduced blocking temperature, T_B/T_o, as a function of the particle size, V/V_o, for different particle concentrations, c/c_o.

The algorithm used for simulations is the same described in Ref. [7].

Results are averaged over 4000–10000 different initial configurations, depending on the particle concentration.

We have selected an arbitrary particle volume, V_o, to express the simulations conditions in reduced units. The temperature is given in reduced units, T/T_o, being $T_o = KV_o/k_B$. T/T_o represents the ratio between the thermal energy and the anisotropy barrier of particles with volume V_o. ZFC curves are obtained increasing the temperature after 100 MC steps in an amount $\Delta T/T_o = 0.005$. The concentration of particles c represents the particle volume fraction in the simulation cell, and $c_o \equiv 2K/M_S^2$ is an adimensional constant.

3. Results

In Fig. 1, the blocking temperature obtained from the peak of ZFC curves is plotted as a function of V/V_o for different particle concentrations. Results have a relatively high error because for moderate and high applied fields or high particle concentrations the maximum is not well defined [7,9,10]. Also, the blocking temperatures at low volumes are less accurate and are subjected to larger calculation errors; so, some deviations at low V/V_o can be observed.

As it is observed, the blocking temperature increases with the particle volume for all concentrations. Two different linear behaviors are showed [10], for small particles ($V < 2V_o$) and bigger ones. For all concentrations, the rate of increase of the blocking temperature with V/V_o is bigger for small particles.

Additionally, the blocking temperature increases, for all V/V_o, with increasing particle concentration. This is the typical behavior observed by different nanoparticle systems [6] and it can be attributed to an increase of the energy barrier when the particle concentration increases.

The slopes obtained from the linear fits are plotted versus the particle concentration c/c_o (Fig. 2). It is observed that the larger the particle concentration c/c_o, the larger the rate of increase of the reduced blocking temperature with the particle size V/V_o. Nevertheless, it tends asymptotically to a constant value for high values of the particle concentration. In other words, the interaction among the particles plays an important role and it seems to saturate for a certain value as we can see in Fig. 2.

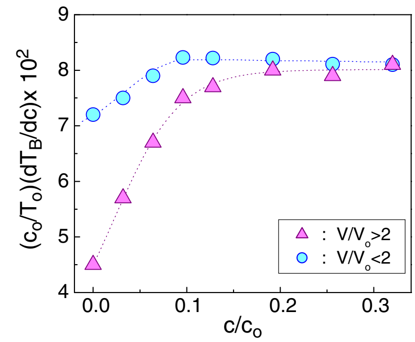

Fig. 2. Slope of the linear fits of Fig. 1 versus particle concentration obtained for small particles (circles) and large particles (triangles). Dot lines are a guide for eyes.

Results seem to indicate that small particles become the saturation to small concentrations than bigger particles and that, for high concentrations, the two different linear regions disappears (the slopes obtained for small and big particles have the same value).

4. Conclusions

For all particle concentrations the reduced blocking temperature obtained from ZFC curves under moderate applied fields increases with the nanoparticle volume and exhibit two different linear regions corresponding to small particles and big particles. The rate of increase is bigger for small particles, and is strongly affected by the interactions between particles (given by the concentration). We observe that the dependence of the blocking temperature with the particle size is bigger the bigger the concentration of particles is, and it tends to a constant value at high particle concentrations. Also, the difference of behavior to small and large particles is negligible for very high concentrations.

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