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Static and Dynamic Properties of Magnetic Nanoparticles with Positive and Negative Uniaxial Magnetic Anisotropy

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To realize a high frequency magnetic material with isotropic magnetic susceptibility, χ, that should be needed for practical high frequency applications such as suppressor of randomly polarized electromagnetic wave noises, we have proposed the magnetic nanoparticles assembly with superparamagnetic properties [1]. According to the thermal relaxation theory, the superparamagnetic properties is maintained up to the blocking resonance frequency, $f_b = f_0\exp(-\Delta EV/k_BT)$. However, because f_0 has some ambiguity, the physical limitation of f_b has not been clarified. In addition, to make the upper frequency limitation of the superparamagnetic properties higher, the influence of the ferromagnetic resonance should be also considered. In this study, in order to clarify the frequency limitation of the superparamagnetic phenomenon, we invcstigated the dynamic responses of the magnetic nanoparticles with positive and negative uniaxial magnetic anisotropy, K_u, by numerical calculation based on Landau-Lifshitz-Gilbert equation where magnetic anisotropy energy, Zeeman energy and thermal energy were considered.

Fig. 1 shows the complex susceptibilities of the magnetic nanoparticles with positive K_u. In the case of $|K_u|V/k_BT >> 1$, the blocking resonances appeared at lower frequency of the theoretical f_r ($=\gamma|H_k|/2\pi$) and ferromagnetic resonance appeared at the theoretical frequency. On the other hand, in the case of $|K_u|V/k_BT << 1$, only the blocking resonance appeared at higher frequency of the theoretical f_r, and the ferromagnetic resonance was not occurred. This result suggests that the upper limitation of superparamagnetic properties of nanoparticles with positive K_u is determined by its f_b and f_b can be increased beyond theoretical value of f_r from H_k by decreasing particle volume.

Fig. 2 shows the complex susceptibilities of the magnetic nanoparticles with negative K_u. In the case of $|K_u|V/k_BT << 1$, only the blocking resonance appeared at higher frequency of theoretical f_r as same as the positive K_u case. However, in the case of $|K_u|V/k_BT >> 1$, both of the blocking resonance and the ferromagnetic resonance appeared at lower frequency of the theoretical f_r from H_k. This result is completely different from the case of positive K_u,

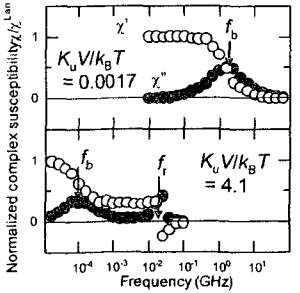

Fig. 1. the frequency dependence of the calculated complex χ of the nanoparticles with H_k of 10 Oe, M_s of 1000 emu/cm^3, T of 300 K.

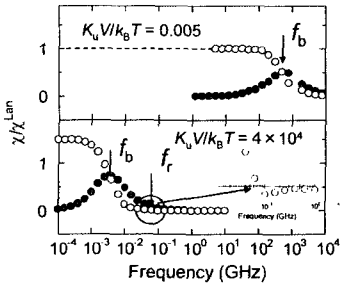

Fig. 2. the frequency dependence of the calculated complex χ of the nanoparticles with H_k of -10 kOe, M_s of 1000 emu/cm^3, T of 300 K.

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QC09

Valence flux under thermal motion in 3D modelling for perovkite manganites

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The visual reconstruction of the valence structure plays an important role in understanding the properties of perovskite manganates at microscopic level. In the $R_{1-x}A_xMnO_3$compounds with a trivalent rare-earths R^{3+}, the Mn^{3+} ions usually exhibit the high spin state $(t_{2g}^3\uparrow, e_g^1\uparrow)$ (S=2) with 10Dq orbital split. Since the egelectrons are responsible for the exchange integral between the manganese ions, the aspect of its density flux is an important factor driving the behaviour of materials. These eg electrons may - despite the strong covalency in the O(2p)-Mn(3d) bonding - split further into two experimentally distinguishable states $e_{x^2-y^2}$ and e_{z^2}. With a substitution of the divalent A^{2+} cations such as Sr^{2+} or Ca^{2+} for R^{3+} a portion of the Mn^{3+} ions is converted into the Mn4+ ions with the high spin ground state $t_{2g}^3\uparrow$ (S=3/2). Thus the number of the remaining $e_g^1\uparrow$ electrons is proportionate to (1-x) per Mn. For the purpose of modelling the thermal flux of the egelectrons, we construct from the original bond-valence-sum equations [1] the multi-dimensional vector fields. For examples, the dynamics of the eg electrons under the symmetric axial vibration in Oh field may be modelled by the following system:

$$\begin{pmatrix} y = 4 - S_{eq} - 2e^{(R_0-R)/B} \\ x = R \end{pmatrix} \qquad (1)$$

where x denotes distance, y denotes the actual number of eg electrons, Seq is the valence sum over 4 equatorial bonds, Rdenotes the apical bonds distance, R0 and B are the empirical constants. Fig. 1 shows the result for the Nd0.5Sr0.5MnO3using the structural parameters taken from [2]. The bond-valence sum method is quite familiar in structural sciences and its application has recently led to the important and beautiful results [3]. This paper shows the other way of using this method in modelling the eg electron flux in the perovskite manganates.

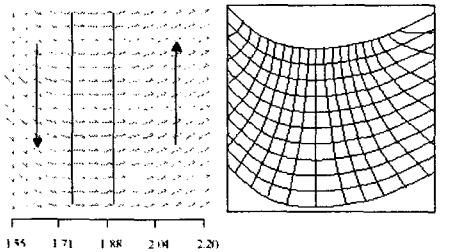

Fig. 1. The e_g electrons vector field. Theleft side shows arrows (contravariants) in 3 different areas of the axial Mn-O bond distance: (1) from 1.55 to 1.78Å, the number of e_g electrons is reducing; (2) from 1.78 to 1.90Å, the atom Mn is in oxidation state 4+ and the number of e_g electrons is near or equal 0; (3) from 1.90 to 2.20Å, the number of $e_g$electrons is increasing (mixed Mn^{3+}/Mn^{4+} state). The right side draws the system of contravariants and covariants, showing the strong bending of the field within the area 1.75-1.95Å of the Mn–O bond distance.

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