

**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,  $\chi$ , 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,  $f_b = f_0 \exp(-\Delta E/k_B T)$ . 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 investigated 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  $|K_u|/k_B T \gg 1$ , the blocking resonances appeared at lower frequency of the theoretical  $f_c (=H_c/2\pi)$  and ferromagnetic resonance appeared at the theoretical frequency. On the other hand, in the case of  $|K_u|/k_B T \ll 1$ , only the blocking resonance appeared at higher frequency of the theoretical  $f_c$ , 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  $f_c$  and  $f_b$  can be increased beyond theoretical value of  $f_c$  from  $H_c$  by decreasing particle volume.

Fig. 2 shows the complex susceptibilities of the magnetic nanoparticles with negative  $K_u$ . In the case of  $|K_u|/k_B T \ll 1$ , only the blocking resonance appeared at higher frequency of theoretical  $f_c$  as same as the positive  $K_u$  case. However, in the case of  $|K_u|/k_B T \gg 1$ , both of the blocking resonance and the ferromagnetic resonance appeared at lower frequency of the theoretical  $f_c$  from  $H_c$ . This result is completely different from the case of positive  $K_u$ .

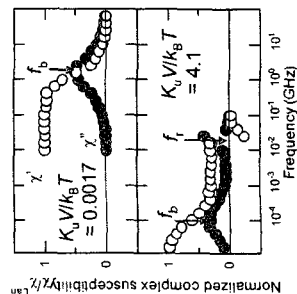


Fig. 1. the frequency dependence of the calculated complex  $\chi$  of the nanoparticles with  $H_c$  of 10 Oe,  $M_s$  of 1000 emu/cm<sup>3</sup>,  $T$  of 300 K.

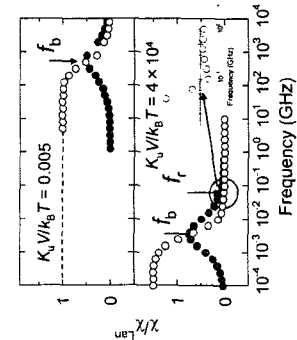


Fig. 2. the frequency dependence of the calculated complex  $\chi$  of the nanoparticles with  $H_c$  of -10 kOe,  $M_s$  of 1000 emu/cm<sup>3</sup>,  $T$  of 300 K.

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**Valence flux under thermal motion in 3D modelling for perovskite manganites**

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The visual reconstruction of the valence structure plays an important role in understanding the properties of perovskite manganites at microscopic level. In the  $R_{1-x}A_xMnO_3$ -compounds with a trivalent rare-earth  $R^{3+}$ , the  $Mn^{3+}$  ions usually exhibit the high spin state ( $t_{2g}^3 e_g^1$ ) ( $S=2$ ) 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  $Mn^{4+}$  ions with the high spin ground state  $t_{2g}^3 e_g^0$  ( $S=3/2$ ). Thus the number of the remaining  $e_g^{\uparrow}$  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:

$$\begin{cases} y = 4 - S_{eg} - 2e^{-(R_0 - R)/B} \\ x = R \end{cases} \quad (1)$$

where  $x$  denotes distance,  $y$  denotes the actual number of eg electrons,  $S_{eq}$  is the valence sum over 4 equatorial bonds,  $R$  denotes the apical bonds distance,  $R_0$  and  $B$  are the empirical constants. Fig. 1 shows the result for the Nd<sub>0.5</sub>Sr<sub>0.5</sub>MnO<sub>3</sub> using 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 manganites.

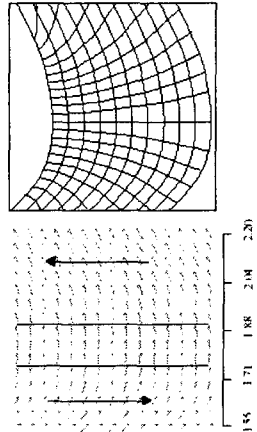


Fig. 1. The  $e_g$  electrons vector field. The left side shows arrows (contravariants) in 3 different areas of the axial Mn-O bond distance: (1) from 1.55 to 1.78Å, the number of  $e_g$  electrons is reducing; (2) from 1.78 to 1.90Å, the atom Mn is in oxidation state 4+ and the number of  $e_g$  electrons 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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