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On the Calculation of Effective Anisotropy Constant of Nanoparticle

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Abstract.A correctcomposition of two kind of magnetic anisotropy of ellipsoidal nanoparticles: crystalline anisotropy and shape anisotropy - has been carried out. It was shown that according to the shape anisotropy the effective anisotropy constant can change non-monotonically. The temperature dependence of effective anisotropy constant on the angle defining the position of effective axis was calculated. It was found out if the angle between thecrystalline anisotropy axis and the long axis of nanoparticle exceeds $\pi/4$, then the effective constant as well as the position of effective axis has to change non-monotonically according to changing of temperature.

Introduction

It's known [1], that metastability or stability of magnetic state depends largely on additional to external field effects, which are reflected in one kind of anisotropy or another (see, for example, [2]). It's the magnetic anisotropy to a large extent determines coercitive force and residual magnetization of magnetic materials using in different devices (magnetic transducers, storage elements, reading devices).

Thereareshapeanisotropy, stress, diffusion, exchange, surface anisotropy and other kinds of anisotropy together with natural crystallineanisotropy and comparable with it in valuecanbefound in a real ferromagnetic. Usually [3-5], effectiveconstantof different kindofanisotropycanbeestimatedas a sumofconstantsof different kindsofanisotropy. As will beshownbelow, such an estimation is rather rough and can essentially influence the effect of characteristics determining one kind of anisotropy or another on effective constant.

Model

- Uniformly magnetizedgrain (single-domain nanoparticle) has a shape of elongated ellipsoid of rotation.
- Magnetic material features uniaxial crystalline anisotropy.
- The axis pointedupbycrystallineanisotropymakesanangle with the long axis of ellipsoid.

Effective anisotropy constantof single-domain ellipsoidal particle

Letusconsidertheanisotropyenergydensityofsingle-domain nanoparticle with neglecting of all other kinds of anisotropy, except of natural crystalline anisotropy and shape anisotropy.

$$E_A = E_A(I_s^2) + \frac{1}{2}\beta_{ik} I_{si} I_{sk} + \frac{1}{2} N_{ik} I_s \quad (1)$$

bythetwicerepeatedindexessumming-

upismeant, β_{ik} and N_{ik} arethetensorsofnaturalcrystallineanisotropyanddemagnetization coefficients which in their principal axes are as follows:

$$\hat{\beta}_{ik} \sim \begin{pmatrix} 0 & \hat{\beta}_{22} & 0 \end{pmatrix}, \ \hat{\beta}_{22} = \hat{\beta}_{33}, \hat{N}_{ik} \sim \begin{pmatrix} 0 & \hat{N}_{22} & 0 \end{pmatrix}. \quad (2)$$

Ingeneralcasetheprincipalaxesoftensors and don'tcoincide,butiteasytoshowthatthereferenceframe (x,)and ($\hat{x}$,), related with principal axes and , can be superposed by means of rotation around the common axis Oz(for an angle ($0 \leq \alpha \leq$). Usingwell-knownlawoftensorcomponenttransformation along with axis rotation, in the frame ($x,$)the total tensor can be written as follows:

$$B_{ik} = \hat{\beta}_{ik} + \tilde{N}_{ik} = \Big(\; (\tilde{N}_{11} - \tilde{N}_{22}) \frac{\sin 2\alpha}{} \qquad B_{22} \qquad 0 \tag{3}$$

$B_{11} = \hat{\beta}_{11} + \tilde{N}_{11} \cos^2 \alpha + \tilde{N}_{22} \sin^2 \alpha,\ B_{22} = \hat{\beta}_{22} + \tilde{N}_{22} \cos^2 \alpha +$ which let us present (1) a follows:

$$E_A = E_A(I_s^2) + \frac{1}{2} B_{ik} I_{si} I_{sk} \tag{4}$$

On summarizing in equation (4) byindexes and , it's easy to obtainthe following formula for calculation of anisotropy energy density:

$$E_A = E_A(I_s^2) - \frac{1}{4} I_s^2 \sin^2 \vartheta \{k_A + k_N + K \cos 2(\varphi - \delta)\} \tag{5}$$

Thefollowingsymbolsareusedhere: ϑ — theanglebetweenthevector $\boldsymbol{I}_s$ andtheaxis z , φ — theanglebetweentheprojectionofvector$\boldsymbol{I}_s$on the planexOyand the axisOx,$k_A = \hat{\beta}_{22} - \hat{\beta}_{11}$($k_A > 0$ — ferromagnetic "light axis" parallel to the axis Ox , $k_A < 0$ — "light plane"), $k_N = \tilde{N}_{22} - \tilde{N}_{11}$($k_N > 0$, if ellipsoid is elongated along the axis,$k_N > 0$if ellipsoid is flattened),

$$\delta = \frac{1}{2} arctg \left(\frac{k_N \sin 2\alpha}{k_A + k_N \cos} \right. \tag{6}$$

$$K = \sqrt{k_A^2 + k_N^2 + 2 k_A k_N \cos}. \tag{7}$$

Thestudyingofformula (5) for the extreme point demonstrate, that $\vartheta =$, φ and $\vartheta =$, $\varphi = \pi$ correspond to minimum, a $\vartheta =$, $\varphi =$; $\vartheta =$, $\varphi = 3\pi/2$ — correspond to maximum of anisotrop yenergy . Thus, the "competition" of crystalline anisotropy and shape anisotropyresults in defining of effective axis, the position of which with respect to the axis is determined by the angle . The formula (7) defines effective anisotropy constant.

Tofindouttheequilibriumstateinthefield it's necessaryto explore the minimum of energy density

$$E = E_A - (H, \boldsymbol{I}_s). \tag{8}$$

For random orientation of vector it's impossible to work out a solution in analytical form. But in the termsof the two special cases **(**is parallel to the plane xOy and is perpendicular to the plane) we can estimate the effect of external field on magnetic states of nanoparticle.

If isparalleltotheplanexOy,thentheanalysisoftheformula (8) brings about the problem of equilibrium states of uniformly magnetized spheroid grain with effective constant , "light axis" of which makes an angle withOx: $K I_s \cos\theta \sin\theta - H_x \cos\theta + H_y \sin\theta$.

It'sresultsfromtheequationthatmagneticmoment of a particle can be either in basic or metastable state. Forcontinuouschangingofmagneticfield theminimalvalueofenergy, corresponding to metastable state comes up toone of the maximal values, and the curve $E = E$instead of extreme point has a point of inflection. Thatistogetherwith $dE/d\theta$ =thesecond-order derivate becomes zero too $d^2E/d\theta^2$ =: $KI_s \cos 2\theta + H_x \sin\theta + H_y \cos\theta$.

Excluding from the two last equations, it's not difficult to work out the formula:

$(H_x)^{2/3} + (H_y)^{2/3} = (KI_s$,whichinvariables and appears to be an astroid equation. Forcriticalfieldtheformulaofirreversibletransitionof magnetic moment of nanoparticle from metastable to the basic state results from above equation:

$$H_c(\Omega) = H_c\left(\sin^{2/3}\Omega + \cos^{2/3}\Omega\right) \tag{9}$$

where Ω istheanglebetweentheeffectiveanisotropyaxisand the vector H , $H_c = I_s\sqrt{k_A^2 + k_N^2 + 2k_A k_N \cos 2\alpha}$ is the maximal critical field.

Theobtainedresultisremarkableduetothefactthatthere is a range of critical fields in a nanoparticles system with different $k_N$andα. Besides, fromthewholesuitofparticleswithsettledangleα, the particles for which the condition$k_N = -k_A \cos 2\alpha$ is met, have the minimal critical field$H_c = k_A I_s \sin 2\alpha$.

Inthesecondcase(is perpendicular to the planexOy)the following equations correspond to minimal energy condition: $\varphi = \delta,\ \pi + \delta,\ \cos\vartheta = 2H/(k_A + k_N + K$,if $H < (k_A + k_N + K)I$and $\varphi = \delta,\ \pi + \delta,\ \vartheta$, if $H \geq (k_A + k_N + K)I$, so the field

$$H_c = \frac{1}{2}(k_A + k_N + K)I_s. \tag{10}$$

Can be named the critical field of reversible rotation of grain's magnetic moment, because when decreasing H to 0 vector $\boldsymbol{I}_s$ willsettle along the "light axis". So, when calculating residual magnetization we have to use the equation(9).

Temperature dependence of critical field of single-domain particle

Non-monotonic temperature dependence of critical field $H_c =$ should be specially marked. Forexample, in the field of temperature, where $(\partial I_s/\partial T)/I_s \ll (\partial k_A/\partial T)$critical field of a grain with settled value of shape anisotropy and $\alpha >$: can have the minimum

$$H_{cmin} = k_N I_s \sin 2\alpha. \tag{11}$$

under the temperature pretemperature, defined with equation

$$k_A(T_{\min}) = -k_N \cos 2\alpha. \tag{12}$$

In the field of temperature, wherethe dependence $I_s$can't be neglected, the condition (12) must be replaced with

$$\frac{dk_A}{dT} I_s \frac{k_A + k_N \cos 2\alpha}{K} + \frac{dI_s}{dT} K \tag{13}$$

Taking into account that the temperature dependence of natural crystalline anisotropy constantis described by the oretic allaw $n(n+1$ [38],we have: $k_A(\ T) = [k_A(T_0)I_s(T)/I_s(T_0$. Usingtheformula $k_A($ it'seasytoshow, thatforparticles with $\pi/2 - (1/2)\arccos(-4/5) \leq \alpha \leq$ critical field becomes minimal.

$$H_{cmin} = k_N I_s(T_{min}) \left[\frac{3}{32}\left(8 - 5\cos^2 2\alpha + 5\cos 2\alpha\sqrt{\cos^2 2\alpha - (4\right.\right. \quad (14)$$

if

$$k_A(T_{min}) = \frac{5}{8}(-\cos 2\alpha + . \quad (15)$$

Withfurthergrowthoftemperaturecriticalfieldincreasesfrom $H_c$to

$$H_{cmax} = k_N I_s(T_{max}) \left[\frac{3}{32}\left(8 - 5\cos^2 2\alpha - 5\cos 2\alpha\sqrt{\cos^2 2\alpha - (\right.\right. \quad (16)$$

whereT_{max}can be defined from the following equation

$$k_A(T_{max}) = \frac{5}{8}\left(-\cos 2\alpha - \sqrt{\cos^2 2\alpha - (4/5)^2}\right)k_N. \quad (17)$$

Particularly, for$\alpha = \pi/2$, $H_{cmin} = 0$, $H_{cmax} = 3\,k_N I_s(T_{max})/4$; T_{min} and $T_{max}$are defined by means of equation$k_A(T_{min}) = k_N$ and $k_A(T_{max}) = k_N/4$.

The position of effective axis also depends on temperature(see(6)). If at the temperature at which anisotropy constant becomes zero, effective axiscoincides with long axis of ellipsoid, then with further temperature changing (growthof k_A) for particlesc $0 \le \alpha \le$:it will monotonically rotate to the axis of crystalline anisotropy, making with it an angle

$$\delta(T) = \frac{1}{2} arctg\left(\frac{k_N \sin 2\alpha}{k_A(T) + k_N \cos 2\alpha}\right). \quad (18)$$

Fornanoparticleswith $\pi/4 \le \alpha \le \pi/2$ growthof $k_A(T)$ at $k_A(T) \le k_N$ results in decreasing of $\delta(T)$ down to $\delta_{min}(T_m) = -\pi/4$. Temperature T_m can be defined from equation$k_A(T_m) + k_N \cos 2\alpha = 0$. Furtherslightincreasingof$k_A(T)$near$T_m$will result in a leap of the angle$\delta(T)$to$\delta_{max}(T_m) = \pi/4$ and then monotonic decreasing along with growth of$k_A(T)$.

Conclusion

Whenadding updifferentkindsofmagneticanisotropyit'snecessarytoconsidertheirtensor nature. Algebraicaddition can be used only if anisotropy axes coincide.

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