GC2024-PERM045

Dependence of the magnetic properties of the metal/metal oxide system on the degree of oxidation

Ilia Iliushin[1], Vladimir Kharitonov[2], Leonid Afremov[1]

[1] Department of Theoretical Physics and Intelligent Technologies, Far Eastern Federal University, Vladivostok 690922, Russia
[2] Laboratory of Spin-Orbitronics, Institute of High Technologies and Advanced Materials, Far Eastern Federal University, Vladivostok 690922, Russia

iliushin.ig@dvfu.ru

The problem of the influence of ferromagnetic metal oxidation on the magnetic properties of the metal/metal oxide system has been the subject of many experimental studies. For example, in [1] it is shown that the oxidation of a thin film of cobalt leads to a decrease in the coercivity and in the saturation magnetisation. A similar dependence of the hysteresis characteristics on the degree of oxidation has been obtained for Co/CoO nanoparticle systems [2]. In [3], a detailed study is presented on the dependence of hysteresis characteristics on the degree of oxidation. The study is devoted to porous films of cobalt nanoparticles that were oxidised in air for more than 1400 hours as a result of controlled annealing at 100°C. The authors have shown that the hysteresis characteristics increase with low oxidation and then decrease with increasing oxidation.

In this work, atomistic modelling of the effect of cobalt oxidation on the hysteresis characteristics of the Co/CoO system has been carried out using cobalt films as an example.

The Landau-Lifshitz-Gilbert equation was used for the atomistic modelling of the magnetisation processes:

$$(\partial \mathbf{S}_i/\partial t)=(\gamma/(1+\lambda^2))(\mathbf{S}_i\times\mathbf{B}^{(\mathrm{eff})}{}_i+\lambda\mathbf{S}_i\times\mathbf{S}_i\times\mathbf{B}^{(\mathrm{eff})}{}_i)$$

where $\mathbf{S}_i$ – spin momentum of the atom, γ – gyromagnetic ratio, λ – the damping parameter, which we have set: $\gamma=1.0$ and $\lambda=1.0$, $\mathbf{B}^{(\mathrm{eff})}{}_i$ – the effective field vector was determined using the Hamiltonian :

$$\mathbf{B}^{(\mathrm{eff})}{}_i=\{B_x=\partial H/\partial S_x,\ B_y=\partial H/\partial S_y,\ B_z=\partial H/\partial S_z\}$$

The Hamiltonian of a Heisenberg spin system is given by:

$$H=-(1/2)\sum_{i,j} J_{ij}S_iS_j - K\sum_i S^2{}_z - \mu_s\sum_i (\mathbf{H},\mathbf{S}_i)$$

the sum of the exchange interaction energies between spin moments with constants J_{ij}, the magnetic anisotropy energy with constant K and the energy of the magnetic moments of the atoms μ_s in an external magnetic field **H** .The study will investigate two models of thin film oxidation: i) layer-by-layer oxidation, where the first monolayer (free surface of cobalt) is oxidised, forming islands that increase in size until complete oxidation of the layer. This process is repeated for the second, third and subsequent layers; ii) combined oxidation, which is a combination of surface and bulk oxidation. The oxidation process begins with the first layer, followed by the formation of cone-shaped structures that sprout layer by layer into the film.

The results of the atomistic modelling of the influence of the oxidation process on the hysteresis properties of Co/CoO films are presented. The dependences of the residual magnetic moment (Mr) (equal to the saturation magnetic moment (M_s)) and coercive force on the relative volume of cobalt oxide $V=V_{CoO}/V_{Co}$ for different oxidation models were calculated. The linear drop in M_s (M_r) was found to be determined by the increase in the relative volume of the oxide in the paramagnetic state for both models. The dependence of the hysteresis characteristics on the degree of oxidation is practically independent of the model used, whether it is layer-by-layer or combined oxidation. It follows from the calculations that the dependence of the hysteresis characteristics on the degree of oxidation is practically independent of the model used.

References:

[1] Tracy, J. B., Weiss, D. N., Dinega, D. P., Bawendi, M. G. Phys. Rev. B. 72(6) pp. 064404, 2005.

[2] Ghoshani, M., Mozaafari, M., Normile, P. S., De Toro, J. A., Al-Nabhani, A. Magnetochemistry. 7(3) pp. 40, 2021.

[3] González, J.A.; Andrés, J.P.; López A, R.; De Toro, J.A.; Normile, P.S.; Muniz, P.; Riveiro, J.M.; Nogués, J. Chem.Mater. 2017, 29, 5200.