Inter-grain exchange interactions for nanocrystalline $Nd_{2.33}Fe_{14}B_{1.06}Si_{0.21}$ magnets

Jin Hanmin*, Wang Xuefeng, Yan Yu, Su Feng

Department of Physics, Jilin University, Changchun 130023, P.R.China

*Corresponding author: e-mail: jhm@mail.jlu.edu.cn, Phone:+86-0431-8499047, Fax:+86-0431-8499073

Abstract

It has been found by this paper's authors that the coercivity $_iH_c$ for nanocrystalline $Nd_2Fe_{14}B$ magnets calculated by the micromagnetics depend on the field directions. The average of the $_iH_c$ calculated along different field directions for a given grain number N decreases with increase of N and approaches a limit $_iH_c(\infty)$. $_iH_c(\infty)$ for small grain diameter D coincide with the experimental values of the nanocrystalline $Nd_{2.33}Fe_{14}B_{1.06}Si_{0.21}$ [1] very well [2-3]. With increase of D, $_iH_c(\infty)$ increases in accordance with the experiments, but the increase is smaller and the discrepancy becomes larger. The difference should be attributed to the neglect of the grain boundary phase in the calculations. In the $Nd_{2.33}Fe_{14}B_{1.06}Si_{0.21}$ magnets, there exists a Nd-rich paramagnetic grain boundary phase, and the thickness of the boundary t=cD (c=const.) increases in proportion to D, thus causing *additional increase in* $_iH_c$. *This work will* evaluate the strength of the inter-grain exchange interaction as a function of t from the differences.

The cubic magnet consists of $n \times n \times n$ (=N) cubic $Nd_2Fe_{14}B$ grains of edge $L(=(\pi/6)^{1/3}D)$. The c-axes of the grains are randomly distributed. Each grain is divided into $m \times m \times m$ cubic regions of edge L/m. For model G, a region is a single domain element exchange coupled with the six adjacent elements. For model S, the region is subdivided into 24 tetrahedral elements of same size, and the magnetic polarization vector $\vec{J}_s$ varies linearly within each element. The periodical boundary conditions of magnetic properties hold for the magnet. By neglecting the stray field energy, the Gibb's free energy of the magnet is the sum of the exchange interaction energy, the magnetocrystalline anisotropy energy and the Zeeman energy. The exchange interaction between the elements across the grain boundary is also formulated by the equation of the exchange interaction between the elements within grain but replacing A by $A\beta$ ($0 \le \beta \le 1$). The applied field is decreased from 5 T by step and the polarization at each field is obtained from a minimization of the energy with respect to the polar angle of polarization at the vertices of the tetrahedral elements.

The strengths of the inter-grain exchange interaction were evaluated for nanocrystalline $Nd_{2.33}Fe_{14}B_{1.06}Si_{0.21}$ magnets by comparing the $_iH_c$ calculated by micromagnetics with the experiments. With increase of the grain diameter from 0 to 10, 30 and 40 nm, the interaction in reference to that without the grain boundary phase decreases to ~ 0.84, ~ 0.57 and ~ 0.40. The interaction extends ~ 0.7 nm deep into the grain, half of the exchange length $\sqrt{A/K_1} \approx 1.3nm$.

References

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