1022, Aq-42

Effect of the shape of grain on the calculated demagnetization curve for nanocrystalline NdFeB magnets

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Abstract

In recent years, many calculations were performed on the demagnetization curves for nanocrystalline Nd-Fe-B magnets by using the micromagnetic finite-element technique [1-4]. If the grain number *N* is taken to be small, the quality of the calculations is not good such as the calculated coercivity ${}_iH_c$ for the stoichiometric composition magnets of different grain sizes *L* are larger than the experimental values for the Nd-rich $Nd_{2.33}Fe_{14}B_{1.06}Si_{0.21}$ magnets [5] by 60-170% [1] in contradiction to that they should be smaller. Griffiths et al simulated the experiments much better by including much larger *N* [2]. It has been found that the calculated curves for the magnet consisting of cubic $Nd_2Fe_{14}B$ grains depend on grain number *N* and the field direction, and the effects are key factors in affecting the quality of the calculation [3]. This paper will study the effect of the shape of grain on the calculated demagnetization curve for nanocrystalline NdFeB magnets.

The cubic magnet consists of $n \times n \times n$ (=N) cubic regions of same dimention. For model A, the $Nd_2Fe_{14}B$ grain is the cubic region. For model B, the $Nd_2Fe_{14}B$ grain is the cubo-octahedron grain which center is the cubic center or vertex of the regions. The c-axes of the grains are randomly distributed to simulate the isotropy of magnet. The periodical boundary conditions of magnetic properties hold for the magnet. By neglecting the stray field energy [4], 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 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 demagnetization curves were calculated for L =10nm and 20nm for model A and L =10nm, 15nm and 20nm for model B. The results reveal that calculated curves, especially that for ${}_iH_c$, is strongly depend on the field direction if magnets consist of small grain number *N*. The range of the difference between the values of ${}_iH_c$ along different filed directions and the average of ${}_iH_c$ decrease with increase of *N*. With increase of *N* to infinity, the average of ${}_iH_c$ approach the limit ${}_iH_c$ ($N=\infty$). J_r/J_S is weakly affected by *N* and the field direction. ${}_iH_c$ ($N=\infty$) and J_r/J_S ($N=\infty$) are almost same for model A and B and coincide with the experimental values of $Nd_{2.33}Fe_{14}B_{1.06}Si_{0.21}$ magnets. The effect of the shape of the grains on the calculated demagnetization curve is small.

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