J. At. Mol. Sci.
doi: 10.4208/jams.053111.071211a

Vol. **3**, No. 3, pp. 218-226
August 2012

Effects of intergranular phase and structure defect on the coercivity for the HDDR Nd–Fe–B bonded magnet

Min Liu[a,*], Xiao-Chen Jin[a], and Ru-Wei Gao[b]

[a] *Department of Electronic Science, Huizhou University, Huizhou 516007, Guangdong, China*
[b] *School of Physics, Shandong University, Jinan 250100, China*

Received 31 May 2011; Accepted (in revised version) 12 July 2011
Published Online 18 February 2012

Abstract. Based on the specific microstructure of HDDR (hydrogenation, disproportionation, desorption, recombination) grains, that the bivariate model concerning the anisotropy constant K_1' and exchange integral A_1' in defect region, which was put forward. Subsequently, the dependence of magnet coercivity on the intergranular phase thickness d and structure defect thickness r_0 was studied. The results showed that the coercivity, H_c, increases with increasing d, for the r_0, the anisotropy constant $K_1(0)$ and exchange integral constant $A_1(0)$ at the grain surface taking different values. While $K_1(0)$ and $A_1(0)$ are fixed, H_c enhances with increasing r_0 for the same d. On the contrary, for the fixed r_0 and d, H_c decreases with increasing $K_1(0)$ or $A_1(0)$. The calculated coercivity is in good agreement with experimental results given by others when d takes 1 nm, r_0 is in the rang of 2–5 nm, $A_1(0)$ and $K_1(0)$ change in the range of (0.6–0.7) of A_1 and K_1, respectively.

PACS: 75.50.Ww, 75.30.Gw

Key words: bonded magnet, bivariate model, microstructure, coercivity

1 Introduction

For the Nd–Fe–B magnet, the magnetic structure parameters will be influenced by the structure defect at the grain boundary. Thus, the crystalline anisotropy constant K_1' the exchange integral constant A_1' and magnetization M_s' in the defect regions of grains are all different from their respective values in the inner part of grains. Usually, three parameters may all vary, and their respective variation laws are different from each other. Most investigators only considered the variation of magnetic structure parameter K_1', which is the main factor influencing the coercivity of magnet, and the other magnetic parameters (A_1',M_s') takes the normal values in the inner part of a grain, respectively. Kronmüller *et al.* [1–3] described

*Corresponding author. *Email address:* `liumin19811001@163.com` (M. Liu)

the anisotropy of defect region by using $K_1' = K_1(\infty) - \Delta K / ch^2(r/r_0)$, where $K_1(\infty)$ is the first crystalline anisotropy constant, ΔK is the reduction anisotropy, r_0 is the defect thickness, and r is the distance to the grain surface. Gao *et al.* [4] used $K_1' = K_1(1 - \exp[-(r/r_0)^2])$ to describe the anisotropy of defect region, where K_1' and K_1 are the anisotropy constant in the inner and boundary parts of a grain, respectively. Both of them investigated the magnetization reversal process and coercivity mechanism of sintered magnet. Liu *et al.* [5] investigated the demagnetization process and coercivity mechanism of HDDR (hydrogenation, disproportionation, desorption, recombination) Nd–Fe–B magnet, by adopting the negative index variation law to describe the anisotropy variation of defect region. Factually, due to the appearance of composition fluctuation and structure defect at the grain boundary, which leads to both crystalline anisotropy constant K_1' and exchange integral constant A_1' may different from their respective values in the inner part of a grain [6]. Theoretically, in order to build an actually simple model describing the microstructures at the grain boundary for the HDDR magnetic powders, then we proposed a bivariate model considering the crystalline anisotropy constant K_1' and exchange integral constant A_1' at the grain boundary region, and further studied the effects of intergranular phase thickness and structure defect thickness on the anisotropy and coercivity of HDDR Nd–Fe–B magnet.

2 Double variable model

The HDDR magnetic powder grain is about $0.2 \sim 0.3$ μm in diameter [7, 8], which is close to the size of a single magnetic domain of $Nd_2Fe_{14}B$ phase, such unique microstructure is between nanocrystalline magnet and sintered magnet. Liu *et al.* [5] considered that the grain boundary anisotropy was simultaneously influenced by the structure defect and exchange-coupling interaction. In this paper, proposed that the HDDR grain is a cubic grain with the edge of 0.3 μm, where the length of exchange-coupling is lex and structure defect thickness is r_0. (Supposed $r_0 > lex/2$, as shown in Fig. 1). And proposed that the intergranular phase is a non-magnetic phase, which distributes homogeneously around the grains. Due to small size of intergranular phase, thus, its thickness d is always smaller than both lex and $2r_0$. The presence of intergranular phase not only weakens the exchange-coupling interaction, but also reduces the region of structure defect at the grain boundary, which leads to the length of exchange-coupling interaction and structure defect thickness reduce from $lex/2$ to $(lex-d)/2$ and from r_0 to $(r_0 - d/2)$, respectively. Based on the different region influenced by the exchange-coupling interaction and structure defect, a grain can be divided the three parts. The center of intergranular phase is chosen as the origin of the coordinate of r. When $d/2 < r < (lex-d)/2$, the anisotropy is simultaneously influenced by the exchange-coupling interaction and structure defect. It is affected by the structure defect alone for $(lex-d)/2 < r < (r_0 - d/2)$. While $r > r_0$, it is not influenced by exchange-coupling interaction and structure defect, and is equal to the K_1 (the normal magnetocrystalline anisotropy constant in the inner part of a grain). Liu *et al.* [5] described the anisotropic variation of defect region by using the variation law of negative index square of r. Han *et al.* [9] pointed out that the variation of