

Comment on “Atomic Origin of Magnetocrystalline Anisotropy in Nd₂Fe₁₄B”

A recent Letter [1] claims to have demonstrated that the strong magnetic anisotropy of today’s best permanent magnet material Nd₂Fe₁₄B is contributed to in a positive way only by one-half of the Nd atoms, namely, by those situated on the 4g sites. The other half, occupying the 4f sites, is alleged to undermine the easy-axis anisotropy. I shall now demonstrate that this conclusion, inferred from magnetic x-ray scattering loops [Fig. 2(a) of Ref. [1]], is mistaken.

At ambient (or higher) temperature the magnetic anisotropy of Nd₂Fe₁₄B is governed by a single crystal field parameter B_{20} , as higher-order terms decay with temperature more rapidly [2]. Therefore, the conclusion of Ref. [1] implies with necessity that B_{20} should be large and negative for Nd(g) while being positive for Nd(f). I have evaluated $B_{20}^{(f)}$ and $B_{20}^{(g)}$, albeit not for Nd₂Fe₁₄B but rather for its close relation Er₂Fe₁₄B, for which sufficient room-temperature neutron diffraction data are available [3]. My results clearly show that both $B_{20}^{(f)}$ and $B_{20}^{(g)}$ are positive in Er₂Fe₁₄B, which corresponds to both of them being negative in Nd₂Fe₁₄B.

Er₂Fe₁₄B is known to undergo a first-order spin reorientation transition at $T_{SR} = 323$ K, where the easy direction of magnetization changes abruptly from [001] to [100]. Accordingly, the magnetic moments of Er above and below the transition point are given by

$$\begin{aligned}\mu_{001} &= (H_{\text{mol}}C/T)(1 - 50.4B_{20}/T + \dots), \\ \mu_{100} &= (H_{\text{mol}}C/T)(1 + 25.2B_{20}/T + \dots)\end{aligned}$$

These are just Eqs. (25) of Boutron [4] adapted for Er ($J = 15/2$, $g_J = 6/5$) in which the role of the applied magnetic field is played by the molecular field H_{mol} . To the considered order in high-temperature expansion the moments are affected only by the second-order crystal field.

Consider the following dimensionless quantity:

$$\frac{\mu_g - \mu_f}{\mu_g + \mu_f} = \begin{cases} \frac{\alpha}{2} - 25.2(B_{20}^{(g)} - B_{20}^{(f)})/T, & T > T_{SR}, \\ \frac{\alpha}{2} + 12.6(B_{20}^{(g)} - B_{20}^{(f)})/T, & T < T_{SR}. \end{cases} \quad (1)$$

Here $\alpha = 2(H_{\text{mol}}^{(g)} - H_{\text{mol}}^{(f)})/(H_{\text{mol}}^{(g)} + H_{\text{mol}}^{(f)})$ is the relative difference between the molecular fields on the two Er sites. These are assumed to depend on temperature similarly to each other, so that α is approximately independent of temperature. Moreover, inelastic neutron scattering on Gd₂Fe₁₄B [5] suggests that α should be small; anything more than a few percent would lead to a detectable line broadening. The smallness of α is essential for the derivation of Eq. (1), which is an expansion in powers of α and $\beta = 1/kT$ taken to linear terms.

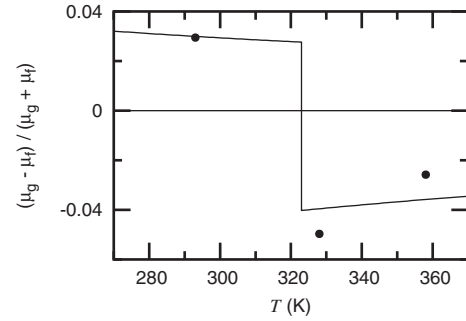


FIG. 1. Temperature dependence of the ratio $(\mu_g - \mu_f)/(\mu_g + \mu_f)$ determined from the neutron diffraction data [3] as well as the best fit to Eq. (1).

Fitting the neutron diffraction data on μ_f and μ_g [3] to Eq. (1) yields $\alpha = 0.01$ and $B_{20}^{(g)} - B_{20}^{(f)} = 0.58$ K, see Fig. 1. So, indeed, $H_{\text{mol}}^{(f)}$ and $H_{\text{mol}}^{(g)}$ differ by as little as 1%.

The average of $B_{20}^{(f)}$ and $B_{20}^{(g)}$ is well known from bulk magnetic measurements: $\frac{1}{2}(B_{20}^{(f)} + B_{20}^{(g)}) = 0.53$ K [6]. Hence in Er₂Fe₁₄B $B_{20}^{(f)} = 0.24$ K and $B_{20}^{(g)} = 0.82$ K.

Summarizing, the available experimental data disprove the statement made in Ref. [1] that $B_{20}^{(f)}$ is opposite in sign to $B_{20}^{(g)}$, at least as far as Er₂Fe₁₄B is concerned. It is therefore most likely that the Nd(f) atoms do contribute positively to the easy-axis anisotropy in Nd₂Fe₁₄B, albeit not as strongly as Nd(g). The origin of the mistake made in the Letter [1] lies in the fact that the magnetic moments of Nd(f) and Nd(g) are regarded as capable of independently taking two different directions to suit their own preferences. In reality, however, the Nd atoms on both sites see a molecular field of an enormous strength, ~ 300 T even at room temperature. By contrast, the anisotropy field is only about 9 T at $T = 300$ K. This means that the Nd moments can deviate from the iron sublattice magnetization vector by mere 0.03 rad (less than 2°). Therefore, the scenario proposed in the Letter [1]—that of two independently reorientating Nd sublattices, one magnetically soft (f) and the other magnetically hard (g)—is physically inconsistent and leads to the wrong conclusion.

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