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MAGNETIC ANISOTROPIES AND SPIN PHASE DIAGRAMS OF $(\text{Pr}, \text{Er})_2\text{Fe}_{14}\text{B}$ AND $(\text{Pr}, \text{Sm})_2\text{Fe}_{14}\text{B}$

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Abstract. - The temperature-composition diagrams, showing the first-order-magnetization-process region, and the spin phase diagrams have been constructed for the $(\text{Pr}, \text{Er})_2\text{Fe}_{14}\text{B}$ and $(\text{Pr}, \text{Sm})_2\text{Fe}_{14}\text{B}$ systems. The magnetic characteristics of both systems can quite well be understood in terms of calculations based on crystalline-electric-field (CEF) theory.

1. Introduction

Both spin reorientation [1] and the first-order magnetization process [2], which occur in some of the $\text{R}_2\text{Fe}_{14}\text{B}$ (R = rare earth) compounds are features from which valuable information on the anisotropy can be deduced. We have reported earlier a systematic study of the influence on the FOMP transition field and on the spin-reorientation temperature of replacement of Pr by Nd [3], which like Pr has a negative second-order Stevens coefficient and thus also has axial preference. Another type of Pr substitution studied is that by Gd [4], which has zero Stevens coefficient. It is also of interest to investigate how the magnetic properties of $\text{Pr}_2\text{Fe}_{14}\text{B}$ are affected if Pr is replaced by rare-earth ions which have positive Stevens coefficients and therefore exhibit planar preference. In the present paper we report the results of studies on two systems in which this type of substitution is realized, $(\text{Pr}, \text{Er})_2\text{Fe}_{14}\text{B}$ and $(\text{Pr}, \text{Sm})_2\text{Fe}_{14}\text{B}$.

2. Experimental details

$(\text{Pr}_{1-x}\text{Er}_x)_2\text{Fe}_{14}\text{B}$ and $(\text{Pr}_{1-x}\text{Sm}_x)_2\text{Fe}_{14}\text{B}$ compounds with $x = 0.0, 0.2, 0.4, 0.6, 0.8$ and 1.0 were prepared by arc-melting, followed by vacuum annealing at 900°C for two weeks. The X-ray diffraction patterns confirmed the compounds to be single phase with the expected tetragonal structure. The powdered specimens used for magnetization measurements were aligned magnetically at room temperature in an external field of about 1 T and fixed in epoxy resin in the shape of cylinders with the long axis either parallel or perpendicular to the magnetic-alignment direction. Magnetization curves up to 20 T were measured at 4.2 K in the High Field Facility at the University of Amsterdam [5] and between 77 K and the Curie temperature in the Magnetism Laboratory of the Institute of Physics in Beijing [6].

3. Results and discussion

From the magnetic isotherms measured with the field perpendicular to the alignment direction the FOMP transition fields, B_{tr} , were determined as the

field corresponding to the starting point of the jump in the magnetization curves. Above 77 K B_{tr} was also determined by means of the Single Point Detection (SPD) method [7]. In figure 1 the temperature dependence of B_{tr} is shown for various compositions. It is clear that B_{tr} decreases with increasing temperature and that Sm substitution depresses the FOMP more than Er substitution. Further, for each compound a critical temperature is found above which no FOMP is observed. These results are depicted in the diagram in figure 2.

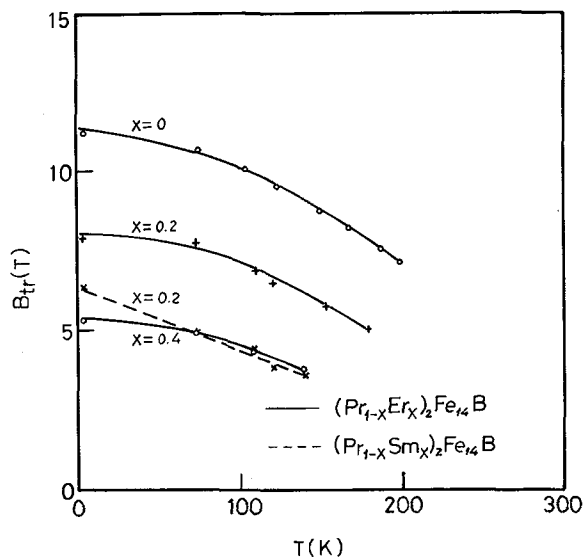


Fig. 1. - The FOMP transition fields of $(\text{Pr}_{1-x}\text{Er}_x)_2\text{Fe}_{14}\text{B}$ and $(\text{Pr}_{1-x}\text{Sm}_x)_2\text{Fe}_{14}\text{B}$ compounds as a function of temperature.

The spin-reorientation temperatures, T_{sr} , were determined by comparing at each temperature the two magnetization curves measured parallel and perpendicular to the c axis, respectively. For $\text{Pr}_{0.2}\text{Er}_{0.8}\text{Fe}_{14}\text{B}$ it is found that below some temperature there is, at least at lower fields, a smaller magnetization if the field is applied parallel to the alignment direction than with the field perpendicular to the alignment direction. This means that below that particular temper-

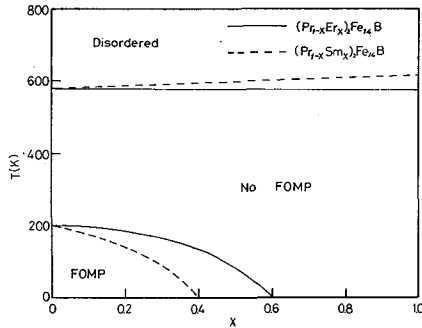


Fig. 2. - The FOMP critical temperature of $(\text{Pr}_{1-x}\text{Er}_x)_2\text{Fe}_{14}\text{B}$ and $(\text{Pr}_{1-x}\text{Sm}_x)_2\text{Fe}_{14}\text{B}$ as a function of x .

ature the easy-magnetization direction has changed from the c axis to the basal plane. Based on such results the diagrams shown in figure 3 have been constructed. By comparing $(\text{Pr}, \text{Er})_2\text{Fe}_{14}\text{B}$ (Fig. 3a) and $(\text{Pr}, \text{Sm})_2\text{Fe}_{14}\text{B}$ (Fig. 3b) it is clear that in the Er-substituted system the spin reorientation is induced by temperature, whereas in the Sm-substituted system it is mainly the composition that determines the spin arrangement.

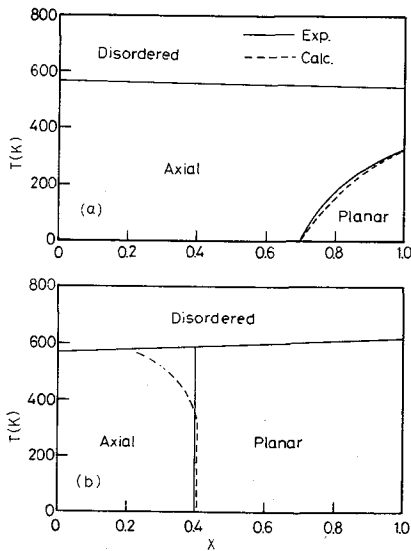


Fig. 3. - Spin phase diagram of (a) $(\text{Pr}_{1-x}\text{Er}_x)_2\text{Fe}_{14}\text{B}$ and (b) $(\text{Pr}_{1-x}\text{Sm}_x)_2\text{Fe}_{14}\text{B}$.

For each ion in the sublattice we have calculated, as a function of temperature, the energy difference Δ between the configuration in which the magnetization is along the c axis and the one with the magnetization in the [100] direction in the basal plane with the following Hamiltonian:

$$\mathcal{H}(\theta, \phi) = \sum_i^{1,2} \mathcal{H}_R(i) + 14K_{\text{Fe}}(T) \sin^2\theta - 14M_{\text{Fe}}(T) \cdot \mathbf{H} \quad (1)$$

$$\mathcal{H}_R(i) = \sum_{n,m} A_n^m(i) C_n^m - 2\mu_B \mathbf{S} \cdot \mathbf{H}_{\text{ex}} + \mu_B (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{H}, \quad (2)$$

where $n = 0, 2, 4, 6$ and $m = 0, \pm 2, \pm 4, \pm 6$. The crystal-field coefficients, A_n^m , were determined by fitting the calculated magnetization curves to the experiments [8]. For $\text{Sm}_2\text{Fe}_{14}\text{B}$ the influence of the excited states has been included. The resultant anisotropy was calculated by using a simple substitution mechanism

$$\Delta(T, \theta) = (1-x) \Delta_{\text{Pr}}(T, \theta) + x \Delta_{\text{R}}(T, \theta), \quad (3)$$

where Δ_{R} is the anisotropy of $\text{R} = \text{Er}$ or Sm in $\text{R}_2\text{Fe}_{14}\text{B}$. The calculated spin-reorientation temperatures as a function of composition are shown by the dashed curves in figure 3 and agree nicely with the experimental results. The anisotropy energies at 0 K obtained in the present calculation are $\Delta_{\text{Pr}} = +160$ K, $\Delta_{\text{Sm}} = -220$ K and $\Delta_{\text{Er}} = -60$ K, in good agreement with the results in [9].

In conclusion we like to emphasize that the magnetic characteristics revealed in both the Er-substituted and the Sm-substituted $\text{Pr}_2\text{Fe}_{14}\text{B}$ can quite well be understood in terms of calculations based on CEF theory.

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