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Spin-reorientation transitions in $RFe_{11}Mo$ (R = rare earth and Y) intermetallic compounds

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Abstract

A series of $RFe_{11}Mo$ compounds (R = Y, Nd, Gd, Tb, Dy, Ho and Er) with the $ThMn_{12}$-type structure have been synthesized. The structural and magnetic properties of the compounds have been investigated by means of X-ray diffraction (XRD) and magnetic measurements. The lattice parameters *a, c* and the unit-cell volume *V* of the compounds decrease with decreasing the atomic radius of the rare earth element due to the lanthanide contraction. The spin-reorientation transition (SRT) was investigated in detail. For $HoFe_{11}Mo$, no SRT was observed. For $NdFe_{11}Mo$, $TbFe_{11}Mo$ and $ErFe_{11}Mo$ one SRT was observed, while for $DyFe_{11}Mo$ two SRTs were observed. By minimizing the magnetocrystalline anisotropy energy, theoretical SR temperatures of the compounds are derived, which show a reasonable agreement with the experimental values.

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Keywords: Rare-earth transition-metal compound; Magnetocrystalline anisotropy; Spin-reorientation transition; $RFe_{11}Mo$ compounds

1. Introduction

Among the rare-earth (R)-transition-metal (T) intermetallic compounds, the $R(Fe,M)_{12}$ (M = transition metal or metalloids) compounds have been widely investigated during the past decades since some of the $R(Fe,M)_{12}$ compounds exhibit various magnetic structures and magnetic anomalies, e.g., first-order magnetization process (FOMP), spin-glass-like transition, spin-reorientation transition (SRT) and magnetohistory effects [1–11]. These compounds crystallize in the tetragonal $ThMn_{12}$-structure with space group I4/mmm. The binary RFe_{12} compounds are unstable and the third element M is needed to stabilize the crystal structure.

In $R(Fe,M)_{12}$ compounds, the Fe-sublattice has been found to exhibit a strong uniaxial anisotropy, while for the rare earth R with negative second-order Stevens factor α_J the R-sublattice shows a planar anisotropy [12]. The contribution of the R-sublattice to the magnetocrystalline anisotropy of the compounds generally dominates at low temperature, whereas that of the Fe-sublattice anisotropy at high temperature. With increasing temperature, the R-sublattice anisotropy usually decreases much faster than the Fe-sublattice anisotropy. Therefore, a temperature-driven SRT could be expected to occur in $R(Fe, M)_{12}$ compounds due to the competition between the anisotropies of the R- and Fe-sublattices [12–14].

The R-sublattice contribution to the magnetic anisotropy energy can be described within the framework of the single-ion crystal-electric-field (CEF) model and the CEF parameters can be determined by fitting different experimental results to the CEF model. Hu et al. [15] have derived a set of five CEF parameters for the Dy^{3+} ion from the analysis of magnetization data of a $DyFe_{11}Ti$ single crystal. By assuming that the CEF coefficients A_{mn} in an isostructural series were approximately constant, the CEF parameters B_{mn} for other R^{3+} were obtained by scaling with appropriate atomic parameters. Using the estimated $B_{nm}(R^{3+})$ and by minimizing the magnetocrystalline anisotropy energy, theoretical SR temperature of other $R(Fe, M)_{12}$ (M = Ti, V, Nb and Si) compounds was

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derived from the temperature dependence of the tilting angle θ between the magnetization and the c-axis. The SR temperatures obtained were in reasonable agreement with experimental observations.

Recently, we reported the magnetic phase diagram of mixed rare-earth $Nd_{1-x}Tb_xFe_{10.5}Mo_{1.5}$ compounds and the change of easy-magnetization direction (EMD) of the compounds from easy cone, via an easy-plane range, to easy-axis with increasing temperature for $x = 0.2$–0.8 [16]. In Ref. [17], we reported the variation of the SRT with nonmagnetic element Y concentration in $Tb_{1-x}Y_xFe_{11}Mo$ compounds. As a systematic research on the spin reorientation of $R(Fe,Mo)_{12}$ compounds, in this paper we investigate the SRT of the $RFe_{11}Mo$ series in detail with R = Y, Nd, Gd, Tb, Dy, Ho and Er.

2. Experiment

Polycrystalline samples of $RFe_{11}Mo$ (R = Y, Nd, Gd, Tb, Dy, Ho and Er) were prepared by arc melting appropriate amounts of the pure metals under high-purity Ar atmosphere. An excess amount of R was added to compensate for the loss during melting and annealing. All the ingots were remelted at least four times to ensure homogeneity. The obtained ingots were wrapped in Ta foil, sealed into evacuated quartz tubes, annealed at 1373 K for 2 weeks, and then quenched in water.

The samples were examined by means of X-ray powder diffraction (XRD) and thermo-magnetic analysis. The XRD data were collected on a Rigaku D/max-2500 diffractometer with Cu Kα radiation and a graphite monochromator. The temperature dependence of the magnetization of the samples was measured in a low field (0.05 T) with a superconducting quantum interference device (SQUID) magnetometer in the temperature range from 5 to 350 K and with a vibrating-sample magnetometer (VSM) from room temperature to above the Curie temperature.

3. Results and discussion

XRD patterns of $RFe_{11}Mo$ (R = Y, Nd, Gd, Tb, Dy, Ho and Er) compounds (Fig. 1) show that all the samples are single phase, crystallizing in the tetragonal $ThMn_{12}$-type structure with the space group I4/mmm, except for a very small amount of Fe phase in $HoFe_{11}Mo$ compound. The lattice parameters a, c and unit-cell volume V derived from the Rietveld refinement of the XRD pattern are listed in Table 1. The a, c and V decrease almost linearly with decreasing atomic radius of the rare earth element due to the lanthanide contraction, as shown in Fig. 2. From Nd to Er, the relative contraction of the c-axis (~0.2%) is much smaller than that of the a-axis (~1.2%). For $YFe_{11}Mo$ compounds, yttrium seems to exhibit a metallic radius between those of terbium and dysprosium, as observed in other yttrium-transition-metal intermetallic compounds with the $CaCu_5$-type derivative structures [18]. Both the

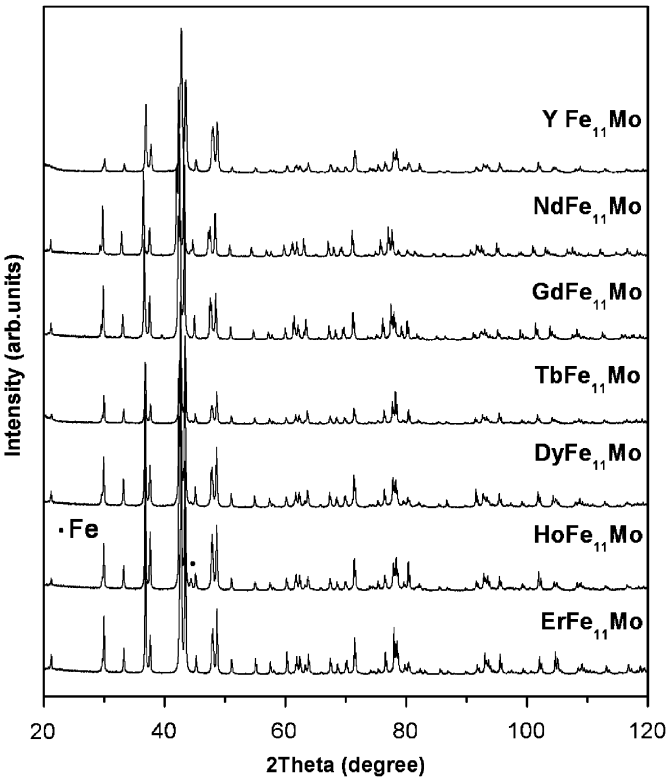

Fig. 1. X-ray diffraction patterns of $RFe_{11}Mo$ (R = Y, Nd, Gd, Tb, Dy, Ho and Er) compounds.

XRD pattern and the observed lanthanide contraction indicate the single-phase character of the synthesized light rare-earth compound $NdFe_{11}Mo$, which used to be prepared by some special processes [19]. As shown below, the Curie temperature of $NdFe_{11}Mo$ is in excellent agreement with the report of Endoh et al. [19].

The temperature dependence of magnetization of RFe_{11}-Mo compounds was measured during warming under 0.05 T after cooling down from room temperature in the applied field (FC). The magnetization curves for $RFe_{11}Mo$ compounds are illustrated in Fig. 3. The curves exhibit some distinct peaks. These peaks correspond to the spin reorientation with increasing temperature. For $DyFe_{11}Mo$, the FC M–T curve exhibits two anomalies in the investigated temperature range, which are associated with the change of the easy magnetization direction from easy plane, via an easy-cone range, to easy axis with increasing temperature [11,12].

Based on the thermo-magnetic measurements, the magnetic phase transition temperatures of the compounds, including the Curie temperature T_C and the spin-reorientation temperature T_{SR}, are determined and listed in Table 1. T_C is obtained by plotting the M^2–T curves and extrapolating M^2 to zero. The spin- reorientation temperature T_{SR} is determined from the peak on the FC M–T curve. The Curie temperature T_C reaches a maximum value for $R = Gd$. As shown in the inset of Fig. 3, for the heavy rare earth (Gd, Tb, Dy, Ho, Er) the T_C increases linearly with the square-root of the de Gennes factor (equivalent to