Magnetic anisotropy in the hexagonal RET_5 compounds

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Abstract

Using the methods of classical statistical mechanics, the field dependence of magnetization curves is calculated at room temperature for $SmCo_5$, $PrCo_5$ and YCo_5. In addition, we discuss the dependence of the magnetization vector on the direction of the magnetic field, along and perpendicular to the easy-axis. We correlate the orientation of the magnetization vector, relative to a specific crystallographic axis, to the angular coordinates of the most probable location in a probability landscape of these anisotropic magnetic systems.

Keywords: Partition function, Anisotropy constant, Probability distribution, Magnetization curves, Saturation magnetization

1. Introduction

Magnetocrystalline anisotropy is one of the intrinsic properties of magnets, which is important in the applications of magnetic materials. As a result, the precisely measured magnetic anisotropy field and anisotropy constants of magnetic materials have long been an important aspect in magnetic research **(Kirchmayr H. R., 1991).**

In the 1960's, hexagonal RCo_5 (R: rare earth) compounds of the hexagonal $CaCu_5$-type made their entry in the world of permanent magnet materials. These permanent magnets RCo5 (e.g with RE= Y, Pr and Sm) have attracted considerable attention due to their large anisotropy fields H_A, relatively high saturation magnetizations M_s and high Curie temperatures T_C. In fact, the first 1 : 5 permanent magnets in the late 1960s were YCo5 magnets **(Kirchmayr H. R., 1996).** At this time, people began to recognize the role of the rare-earth anisotropy and that led to the discovery of samarium–cobalt magnets by Karl J. Strnat et al. in 1967**(Strnat K. J. et al., 1967)**. SmCo5 compound is successfully fabricated into high energy permanent magnets due to its exceptionally high energy product and large coercivity, in addition to its high Curie temperature. It has very large Magnetocrystalline anisotropy constant, $1.7x10^8$ erg/cm^3 at 300 K **(Das D. K., 1969; Sayama J., 2004).** PrCo5 and YCo5 also have attracted attention for their good magnetic properties. The PrCo5 compound has a higher theoretical energy product (39 MGOe) than the SmCo5 compound and the element Pr is more abundant in nature than Sm **(Shen Y. et al.,1991).** Rare-earth-cobalt permanent magnets materials have important applications and the most important one is to provide a static magnetic field of specified strength in a designated space such as in magnet motor, magnet generator, magnetic resonance imaging, loudspeaker, actuator, magnetic separator, traveling wave tube, eddy current brake, etc **(Strnat K. J., 1990).**

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2. Materials and Methods

The classical statistical physics are appropriate for treating the magnetization vector as a classical vector. The angular states, of such a vector should assume continuous, rather than discrete values, i.e. the polar and azimuthal angles θ_m and φ_m should have all continuous values in their respective ranges 0–π and 0–2 π, respectively and hence integration rather than summation should be used.

The classical partition function is given by

$$Z = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} e^{-\beta EV} \sin\theta_m \, d\theta_m d\varphi_m \tag{1}$$

where V is the volume of a spherical magnetic particle (where r =80 Å in radius) throughout this work and $\beta = 1/k_B T$, where k_B is the Boltzmann constant and T is the absolute temperature. E is the total energy density of this hexagonal magnetic system. The total energy, however, may include other types of energy e.g. magnetostrictive for specific systems, but in the present work we focus only on the magnetocrystalline anisotropy, besides of course, the Zeeman term, therefore the energy density takes the following form:

$$\mathrm{E_K} = \mathrm{K_1} \sin^2 \theta_m + \mathrm{K_2} \sin^4 \theta_m - HM_s(\cos\theta_m \cos\theta_h + \sin\theta_m \sin\theta_h \cos(\varphi_m \varphi_h) \tag{2}$$

where K_1 and K_2 are the anisotropy constants, M_s is the saturation magnetization, θ_m is the polar angle of the magnetization direction with respect to the c-axis, φ_m is the azimuthal angle of the magnetization direction with respect to the easy-axis in the basal plane, θ_h is the angle between the magnetic field H and the *c*-axis, φ_h is the azimuth angle of H in the basal plane **(AiMin W. and Hua P., 2009; Sobh H. A. et al., 2014).** There exist three kinds of magnetocrystalline anisotropy in hexagonal compounds according to the signs and magnitudes of K_1 and K_2: uniaxial c-axis anisotropy, basal-plane anisotropy and easy-cone anisotropy. We should emphasize that a more complete form of anisotropy energy contains more than two anisotropy constants, in addition to terms which are φ_m dependent. But we deal in the present paper with only two anisotropy constants and therefore our expression of the anisotropy energy has no φ_m dependence. The φ_m dependence shows up in the Zeeman term.

The magnetization, at constant T, is calculated using the following relation:

$$M = \frac{1}{\beta} \frac{\partial \ln Z}{\partial H} \tag{3}$$

The probability, for the magnetization vector, to have an angular coordinate θ_m , at a given temperature and field is given by

$$P = \frac{e^{-\beta EV}}{Z} \tag{4}$$

Studying the probability angular dependence is important for an understanding of the behavior of magnetic systems.

We have used the cgs system of units and the Mathematica software package for numeric, symbolic, fitting analysis and plotting our results throughout the present work (www.Wolfram.Com).

3. Results and discussion

3.1. The magnetization curves

We will discuss here specific features of magnetization curves calculated by using our method. Table 1 show the values of K_1, K_2 and M_s that we used **(Chen C., 2010; Tatsumoto E. et al. ,1971).** As shown in Fig.1, 2 and 3, the magnetization increases rapidly with the applied field along the c-axis and attains saturation very fast. This axis, therefore, is called the easy axis since the magnetization is easily saturated along which. But when the field is applied along any other direction, in the basal plane, the magnetization increases at a constant rate, but attain less values, at the same field, compared to the easy direction, until it saturates at the same value as for the easy axis (H_A) . Since it is more difficult to saturate the magnetization along this axis, it is called the hard axis of magnetization.

Table 1 Saturation magnetization and anisotropy constants of $PrCo_5$, $SmCo_5$ and YCo_5.

	M_s emu/cm^3	K_1 10^7erg/cm^3	K_2 10^7erg/cm^3
$PrCo_5$	955	9.77	0.05
$SmCo_5$	910	17	0
YCo_5	844	5.5	0.02

In Fig.1, we can see that $PrCo_5$ reaches saturation in the hard direction at anisotropy field of 210 kOe, while $SmCo_5$ at 360 kOe and YCo_5 at 140 kOe. These results are in good agreement with the experimental results **(Strnat K. J., 1988; Hoffer G. and Strnat K. J., 1966; Kirchmayr H. R., 1991; Kirchmayr H. R., 1996 and Dreyer S. et al., 2007),** see Table 2.

Table 2 Comparison between experimental and theoretical results.

	H_A (kOe) Experimental results	H_A (kOe) Theoretical results
$PrCo_5$	200	210
$SmCo_5$	300	360
YCo_5	130	140

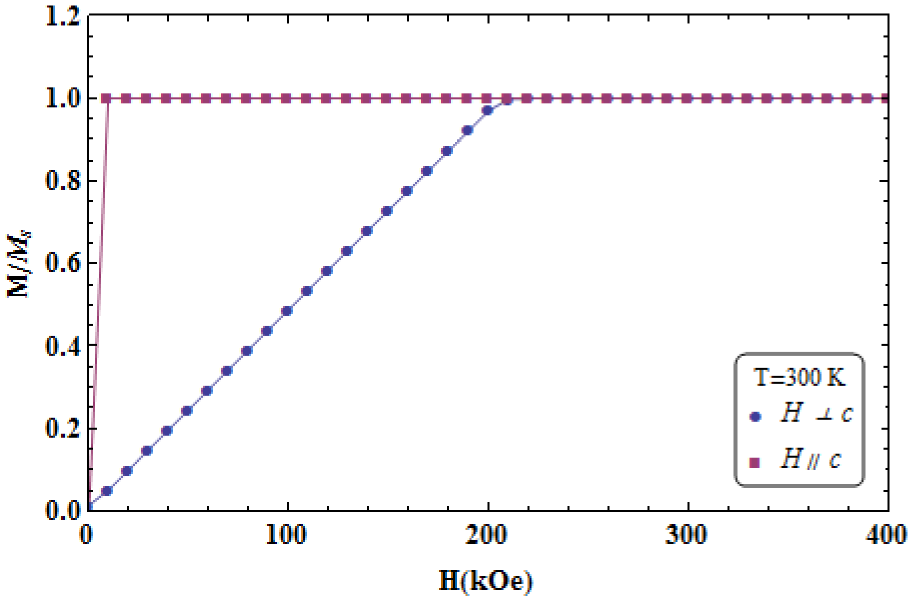

Figure 1 The magnetization curves of $PrCo_5$ along and perpendicular to the c-axis at 300 K.

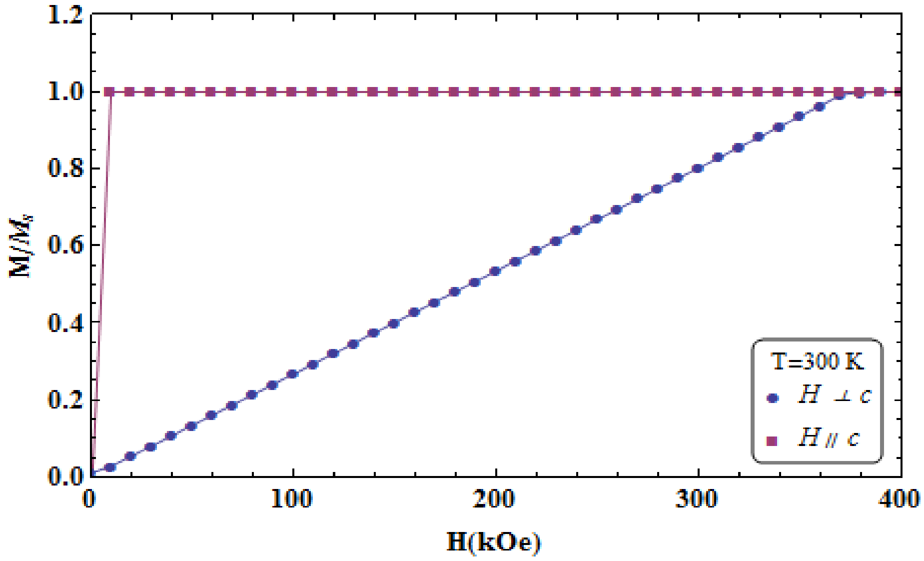

Figure 2 The magnetization curves of $SmCo_5$ along and perpendicular to the c-axis at 300 K.

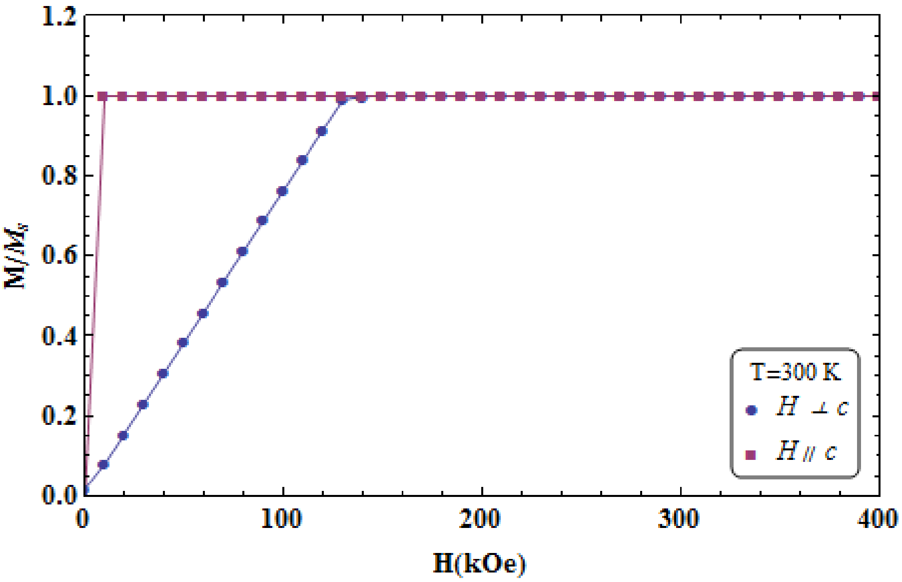

Figure 3 The magnetization curves of YCo_5 along and perpendicular to the c-axis at 300 K.

3.2. The probability landscape

The evolution of the angular coordinates of a probability peak upon changing the magnetic field, at a given temperature, sheds light on the magnetization process in this anisotropic system. We study here the probability and energy landscape for $SmCo_5$ when the field is along eather the c-axis or and in the basal plane at room temperature.

First, at zero field (H=0), the probability has one maximum at θ_m =0 rad for all values of φ_m (Fig.4) which means that the magnetization is totally aligned along the c-axis in the absence of the external field, Fig.4. The corresponding energy landscape also at H=0 is shown in Fig.5. It is evident that the energy minimum is located at θ_m =0, i.e. where the probability maximizes.

When the external field is exist along the c-axis, the probability peak will increase which means that the magnetization vector alignment along c-axis increase with field. The probability landscape at H=30 kOe is shown in Fig.6.

Now when the field is applied within the basal plane (H=300 kOe), the probability appears in a small peak at θ_m =2.5 rad, Fig.7. The energy landscape shows a minimum also at the same value at which the probability maximizes (Fig.8). This value however is still far from 1.5 rad (i.e. 90 degrees) which is the location of the basal plane. This means that the uniaxial anisotropy is so strong to lock the magnetization vector along the c-axis even at this high field.

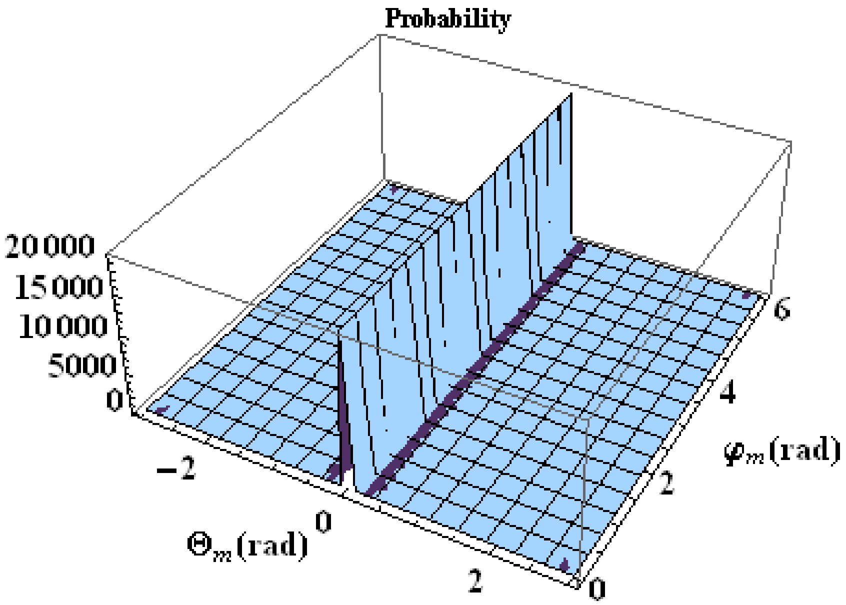

Figure 4 The probability landscape of $SmCo_5$ at T=300 K and zero field along the c-axis.

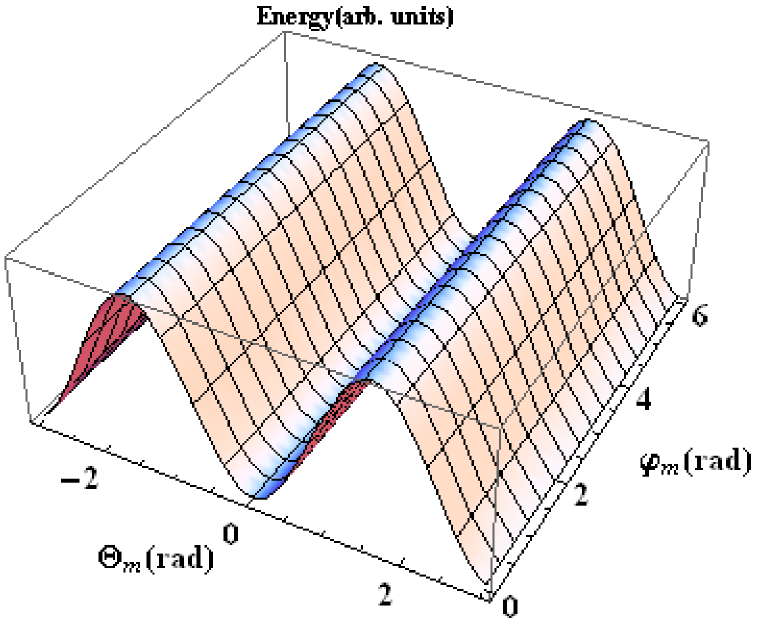

Figure 5 The energy landscape of $SmCo_5$ at T=300 K and zero field applied along the c-axis.

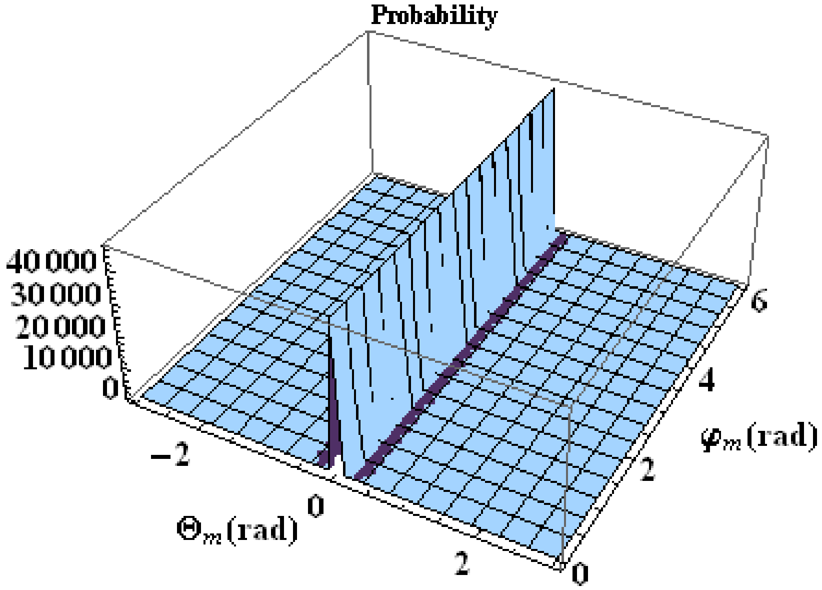

Figure 6 The probability landscape of $SmCo_5$ at T=300 K and H=30 kOe along the c-axis.

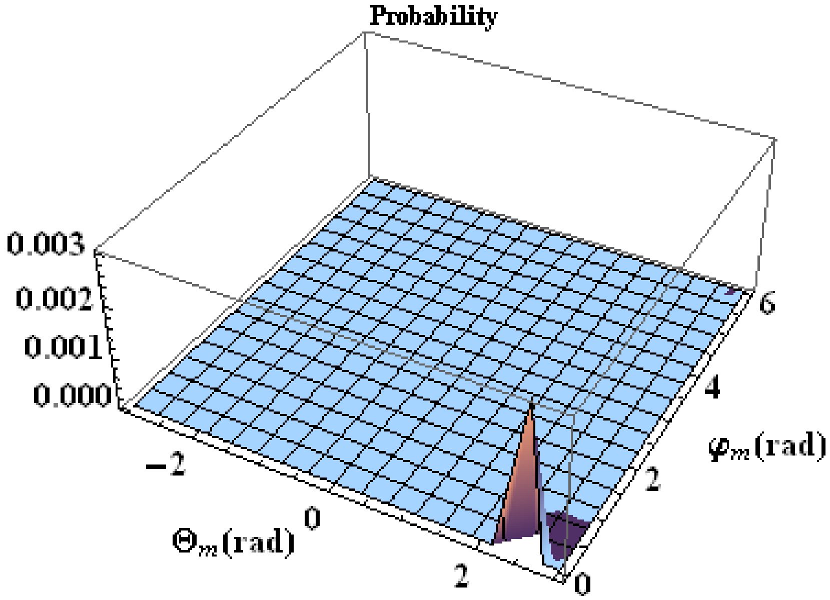

Figure 7 The probability landscape of $SmCo_5$ at T=300 K and H=300 kOe field perpendicular to the c-axis.

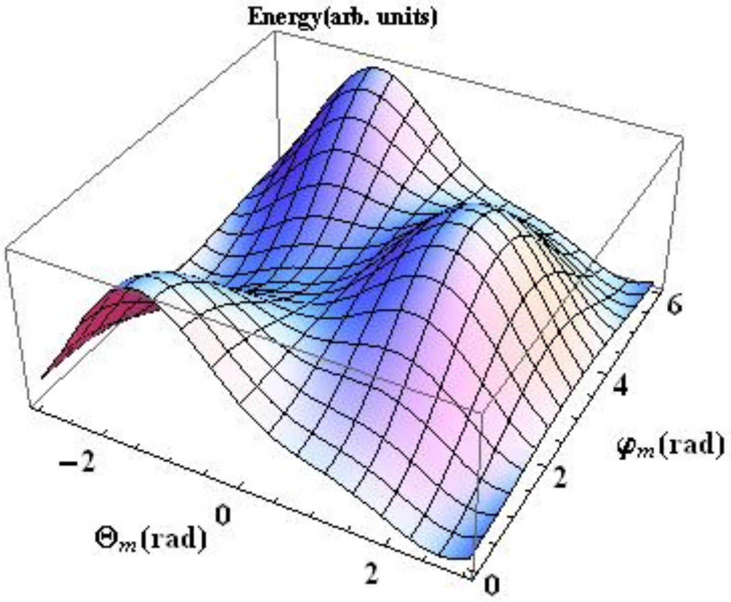

Figure 8 The energy landscape of $SmCo_5$ at T=300 K and H=300 kOe perpendicular to the c-axis.

4. Conclusions

The fundamental assumptions and the methods of statistical mechanics seem to present consistent results for the magnetization curves of three different REO_5 compounds with RE= Y, Pr and Sm. The changes and alignment of the magnetization vector along field direction at room temperature is discussed. The evolution of the most probable orientation of the magnetization vector with magnetic field strength and direction is interpreted in terms of energy minimization. Our results are in good agreement with some available experimental results.

5. References

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الملخص باللغة العربية

التباين المغناطيسي في مُركبات RET_5 ذات البنية البلّورية السداسية

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باستخدام طرق الميكانيكا الاحصائية الكلاسيكية، تم حساب منحنيات بين المجال المغناطيسي و المغنطة عند درجة حرارة الغرفة للمركبات $SmCo_5$, $PrCo_5$ و YCo_5 . أيضا ناقشنا اعتماد متجهه المغنطة على اتجاه المجال المغناطيسي، سواء في اتجاه المحور السهل أو عمودي عليه. تم ربط توجه المتجه المغناطيسي بالإحداثيات الزاوية للموقع الأكثر احتمالا في مشهد الاحتمالات في هذه الأنظمة المغناطيسية متباينة الخواص.