

# Relation between stabilization energy, crystal field coefficient and the magnetic exchange interaction for $Tb^{3+}$ ion

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**Abstract:** Based on a single ion model, Hamiltonian of the simplest form about magnetocrystalline anisotropy for  $Tb^{3+}$  ion was solved by using the numerical method. The relation between the stabilization energy, crystal field coefficient  $B_2^0$  and the magnetic exchange interaction was studied as temperature approaches to 0 K. The results show that the stabilization energy contributed by  $Tb^{3+}$  is linear with crystal field coefficient  $B_2^0$  approximately, but it is insensitive to the change of magnetic exchange interaction for the strong magnetic substances such as  $TbCo_5$ ,  $Tb_2Co_{17}$  and  $Tb_2Fe_{14}B$  compounds.

**Key words:** single ion model; magnetic exchange interaction; crystal field coefficient; stabilization energy

## 1. Introduction

In the early 1970s, Greedan and Rao[ 1] had calculated the simplest Hamiltonian based on the magnetocrystalline anisotropy single ion model using the numerical method and presented the relation between the easy magnetization direction (the easy plane or the easy axis) of rare earth magnetic sublattice and the sign (positive or negative) of crystal field coefficient  $B_2^0$  for  $RCO_5$  (R= rare earth) and  $R_2Co_{17}$  compounds. On these, the experimental facts of the easy magnetization direction were interpreted for the compounds. Moreover, this method is suitable for other strong magnetization compounds under the allowable condition of ignoring all terms of crystal field coefficient except  $B_2^0 O_2^0$ . Large numbers of reports show that single ion model explains the magnetocrystalline anisotropy of 4f ion in the rare earth compounds successfully[ 2-4].

When the easy and hard magnetization direction along the axis or the plane, the stabilization energy of  $R^{3+}$  ion takes the maximum or the minimum of the magnetocrystalline anisotropy

energy attributed by the  $R^{3+}$  ion[ 1]. The main form of the Hamiltonian only contains the crystal field action and magnetic exchange interaction when employing single ion model to calculate the magnetocrystalline anisotropy energy of 4f-ion in rare earth transition-metal intermetallic compounds. The crystal field coefficient can be obtained from magnetization measure or calculation, but there is definite deviation. Magnetic exchange interaction estimated by molecule field approximation also exists deviation about 30% [ 5-7]. So it should be a significant research to identify the effect on the magnetocrystalline anisotropy by changing crystal field coefficient and magnetic exchange interaction. In this paper, adopting a single ion model, the simplest Hamiltonian of magnetocrystalline anisotropy of  $Tb^{3+}$  ion was calculated by numerical method. The relation between the stabilization energy, the crystal field coefficient and magnetic exchange interaction was presented under the action of various crystal field and molecule field.

## 2. Calculating method

According to the single ion model, the

Hamiltonian acting on the ground-state wave function of rare earth ion can be written as follows:

$$H = \sum_{n,m} B_n^m O_n^m + 2(g_J - 1) \mu_B J \cdot H_{ex} \quad (1)$$

The first term of Eq. (1) is the generalized formulation of crystal-field interaction and the second represents the interaction of the rare earth magnetic moment with the exchange field. For the first-grade approximation, Hamiltonian can be expressed in the simple form:

$$H = B_2^0 O_2^0 + G(J_x \sin \theta + J_z \cos \theta) \quad (2)$$

here,  $G = 2(g_J - 1) \mu_B H_{ex}$ ,  $O_2^0 = 3J_z^2 - J(J+1)$ . Where  $B_2^0$  is crystal field coefficient,  $O_2^0$  is the Stevens equivalent operator [8-9],  $H_{ex}$  represents intensity of exchange field acting on the rare earth sublattice.  $J$ ,  $J_x$ ,  $J_z$  are total angular momentum and its component of R<sup>3+</sup> ion respectively, and  $\theta$  is the angle between  $H_{ex}$  and the  $c$ -axis.

For Tb<sup>3+</sup> ion,  $J = 6$ , select values of  $B_2^0$  and  $G$ , then act Eq. (2) on the ground-state wave function of Tb<sup>3+</sup> ion and adopt numerical method, thirteen splitting values  $E_i(\theta)$  ( $i = 1, 2, 3, \dots, 13$ ) can be obtained. According to the free energy expression given by Helmholtz, the magnetocrystalline anisotropy energy of Tb<sup>3+</sup> ion is:

$$E_{an}(\theta, T) = -kT \ln \sum \exp[-E_i(\theta)/kT] \quad (3)$$

Stabilization energy:

$$E_{st}(T) = E_{an}(90^\circ, T) - E_{an}(0^\circ, T) \quad (4)$$

As  $T \rightarrow 0$  K,

$$E_{st}(0) = E_{an}(90^\circ) - E_{an}(0^\circ) \quad (5)$$

### 3. Results and discussion

From Eqs. (2) - (5), the numerical relation between  $E_{st}$  and  $B_2^0$  can be obtained by given values of  $G$  arbitrarily as  $T \rightarrow 0$  K. Similarly, relation between stabilization energy and magnetic exchange interaction can be obtained by given values of  $B_2^0$  arbitrarily. For advantage of analysis, some results are plotted in Figs. 1 and 2.

Just as shown Figs. 1 and 2, for different  $G$ ,  $E_{st} > 0$  as  $B_2^0 < 0$ , which implies the easy

magnetization direction of Tb lattice is parallel to  $c$ -axis; but  $E_{st} < 0$  as  $B_2^0 > 0$ , which expresses the easy magnetization direction is perpendicular to  $c$ -axis. The results show quite good agreement with those obtained by Greedan and Rao [1].

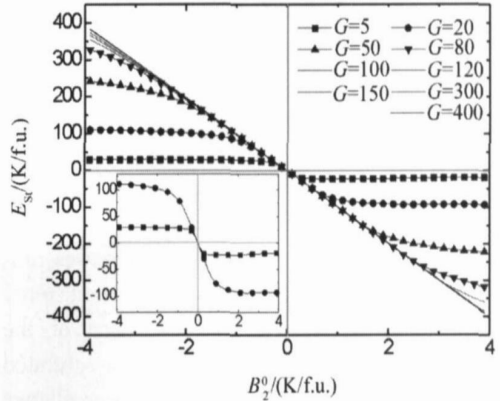


Fig. 1. Relation between stabilization energy and crystal field coefficient for given  $G$  (K/f. u.). (1 K can be converted to  $1.381 \times 10^{-23}$  J).

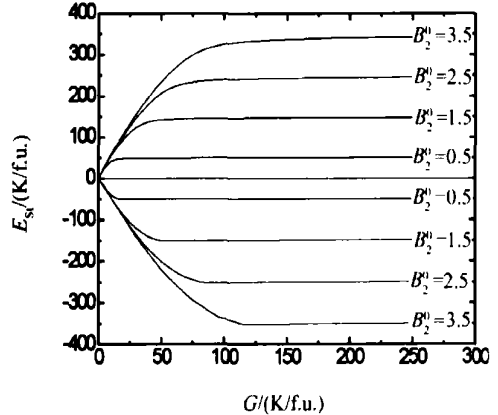


Fig. 2. Relation between stabilization energy and magnetic exchange interaction for given  $B_2^0$  (K/f. u.).

Fig. 1 displays the variations of stabilization energy with crystal field coefficient for  $G = 5, 20, 50, 80, 100, 120, 150, 300, 400$  K/f. u. . From Fig. 1, the variety of stabilization energy of Tb<sup>3+</sup> ion with crystal field coefficient  $B_2^0$  is very complex and does not exhibit any clear simple functional relations when values of  $G$  are lower. The smaller graph embedded in Fig. 1 shows details of variation stabilization energy with crystal field coefficient for  $G = 5$  K/f. u., 20 K/f. u. When values of  $G$  are

higher (such as  $G > 80$  K/f. u.), stabilization energy of  $Tb^{3+}$  ion is linear with crystal field coefficient  $B_2^0$  approximately, showing as the curves when  $G = 100, 120, 150, 300, 400$  K/f. u. in Fig. 1. More calculations indicate  $E_{st}/B_2^0 \approx \text{constant}$  as  $G > 80$  K/f. u.

Fig. 2 displays the changing curves of stabilization energy with magnetic exchange interaction when  $B_2^0 = \pm 0.5, \pm 1.5, \pm 2.5, \pm 3.5$  K/f. u. For any curve in Fig. 2, the whole changing range for values of  $G$  can be divided sketchily into three regions according to the variety of stabilization energy: (a) non-saturated region, stabilization energy increases rapidly with increasing  $G$  from the start of zero, with further increasing  $G$ , the slope of the curve decreases gradually; (b) quasi-saturated region, more bigger of  $G$ , more slower change of stabilization energy; (c) saturated region, when values of  $G$  increase further, stabilization energy do not exist obvious changing pattern. If the  $G$  at which the stabilization energy reaches 95% of its maximum is defined as the left boundary of quasi-saturated region, then the dependence of stabilization energy on  $G$  is weak in the quasi-saturated region and saturated region for any curve. In addition, it can be seen from Fig. 2, smaller the  $|B_2^0|$  is, smaller the corresponding non-saturated region is.

For strong magnetic substance,  $TbCo_5$  ( $B_2^0 = 1.4$  K/f. u.,  $G = 210$  K/f. u.) [1],  $Tb_2Co_{17}$  ( $B_2^0 = 0.43$  K/f. u.,  $G = 210$  K/f. u.) [1],  $Tb_2Fe_{14}B$  ( $B_2^0 = -2.4$  K/f. u.,  $G = 152$  K/f. u.) [10], values of  $G$  of  $Tb^{3+}$  ion are in quasi-saturated region or saturated region, so the variation of stabilization energy of  $Tb^{3+}$  ion is linear with crystal field coefficient  $B_2^0$  approximately, but the variation of magnetic exchange interaction has no obvious effect on the stabilization energy.

#### 4. Conclusions

As temperature approaches to 0 K, for weak magnetic substances, the variety of stabilization energy of  $Tb^{3+}$  ion with crystal field co-

efficient  $B_2^0$  and magnetic exchange interaction is more complex. But for strong magnetic substances, variation of stabilization energy of  $Tb^{3+}$  ion is linear with crystal field coefficient  $B_2^0$  and insensitive to the change of magnetic exchange interaction.

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