

## Neutron diffraction study of the magnetic structure of erbium

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The magnetic structure of high-purity single crystals of erbium has been studied by neutron-diffraction techniques. Although the general characteristics of the magnetic structure of erbium have been found to be in agreement with earlier measurements, several interesting new features have been observed. At 84.4°K the  $c$ -axis moment orders in a sinusoidally modulated magnetic structure with wave vector along the  $c$  axis, and develops higher-order harmonics as the temperature is decreased below the Néel point. The third- and fifth-order modulations of the  $c$ -axis moment were of measurable intensity at temperatures as high as 75 and 55°K, respectively. Higher-order harmonics up to the 17th order have been observed as the temperature was decreased down to 22°K. At 52.4°K the basal-plane moment was found to order in a spiral with wave vector equal to that of the  $c$ -axis moment. Third- and fifth-order harmonics of the basal-plane moment were observed between approximately 50 and 18°K. At 18°K a transition to a ferromagnetic spiral structure was observed; significant hysteresis effects were observed in the vicinity of this transition temperature. Significant short-range-order effects have been observed above the Néel and the basal-plane-ordering temperatures. The temperature dependence of the wave vector of the magnetic structure was found to exhibit a number of anomalies associated with commensurability of the magnetic periodicity with that of the lattice. The basic features of the temperature dependence of the wave vector are in good agreement, in the (84–18)°K temperature region, with the Elliott-Wedgewood theory. The temperature dependence of the  $c$ - and  $a$ -axis lattice constants has been measured and found to exhibit significant magnetostriction effects.

### I. INTRODUCTION

The first neutron-diffraction investigation of the magnetic structure of erbium was performed by Cable, Wollan, Koehler, and Wilkinson.<sup>1</sup> These measurements revealed the existence of three distinct regions of long-range order: (i) the high-temperature region [(80–52)°K], in which the  $c$ -axis moment orders in a purely sinusoidal magnetic structure with wave vector parallel to the  $c$  axis; (ii) the intermediate temperature region [(52–20)°K], in which the basal-plane moment orders in a spiral and a third-order modulation along the  $c$  axis is observed; (iii) the low-temperature region [(20–4.2)°K], in which the magnetic structure is a ferromagnetic spiral.

Recent measurements<sup>2–4</sup> of the magnetic susceptibility of erbium showed anomalies in the vicinity of 28°K and 35°K. At approximately 28°K, anomalies were also observed in specific-heat,<sup>5</sup> resistivity,<sup>6</sup> and thermal-conductivity measurements.<sup>7</sup> In order to determine whether these anomalies are associated with new magnetic structures, a neutron-diffraction investigation was initiated using single crystals of considerably greater purity than the ones used in the earlier investigation,<sup>1</sup> particularly with regard to nonmetallic elements.

### II. EXPERIMENTAL DETAILS

Single crystals of erbium have been grown by the strain-anneal technique<sup>6,8</sup> from high-purity material prepared in this Laboratory. The over-all purity of the crystal used in the present experi-

ment was found to be better than 99.9 at.%, and the highest detected impurity content was that of O with 116 ppm by weight of Er metal. The concentration of individual impurities in the crystal is given in Ref. 2. The crystal was a pillar of rectangular cross section with dimensions of approximately 1×1×6 mm. The crystal was cut with the ( $h0l$ ) plane of the reciprocal lattice perpendicular to the long axis of the pillar.

Intensity measurements performed with single crystals must be corrected for secondary-extinction effects. In the case of erbium, where the intensities of the various nuclear and magnetic diffraction peaks differ by several orders of magnitude, the correction for secondary extinction effects may introduce a considerable uncertainty in the calculated moments. In order to minimize this problem the mosaic spread of the sample was increased gradually by successive compressions of the crystal. After each compression, the mosaic spread of the crystal was assessed by measuring the full width at half-maximum (FWHM) of the (004) reflection of Er, using a monochromatic neutron beam obtained by reflection from the (400) planes of a perfect Ge crystal. The crystal was compressed until its FWHM increased from 2 to approximately 17 min of arc. The absence of any appreciable secondary extinction effects was assessed by measuring the integrated reflectivities of the (100), (200), (300), (400), (002), (004), (006), (008), (101), and (202) nuclear reflections at room temperature. The measured integrated reflectivities, corrected for absorption, were consistent

with negligible secondary extinction and a Debye-Waller correction corresponding to a Debye temperature of  $(181 \pm 5)^\circ\text{K}$ . The conclusions, regarding the secondary extinction and Debye-Waller corrections, were checked by two independent measurements. The integrated reflectivities of the nuclear reflections were compared at liquid- $\text{N}_2$  and liquid-He temperature. The Debye temperature obtained from these measurements agreed, to within experimental precision, with that obtained from the room-temperature measurements. In addition, the magnetic form factor of Er was measured at liquid-He temperature and found to be in good agreement with previous measurements of the  $\text{Er}^{3+}$  form factor by Cable *et al.*<sup>1</sup> and Koehler and Wollan.<sup>9</sup>

The measurements were performed using a double-axis neutron diffractometer at the Ames Laboratory Research Reactor. The neutron wavelength  $\lambda$  was  $1.05 \text{ \AA}$  with a  $\frac{1}{2}\lambda$  contamination of approximately 0.6%. The intensity measurements were performed, in the  $(6-95)^\circ\text{K}$  temperature region, with the crystal oriented so that the  $(h0l)$  plane of the reciprocal lattice coincides with the scattering plane. Below  $50^\circ\text{K}$  the sample temperature was measured using a calibrated Cu-Au (0.03-at.% Fe) thermocouple, and above this temperature with a calibrated Cu-Constantan thermocouple. The temperature was controlled to within  $0.1^\circ\text{K}$  by a second pair of thermocouples.

At every temperature the positions of the magnetic satellites were obtained by scanning the  $(h0l)$  plane of the reciprocal lattice along lines parallel to the  $[00l]$  direction. The positions of the satellites were determined by taking the centers of gravity of the neutron peaks. The wave vector  $q$  of the magnetic periodicity was obtained by taking the average of the  $q$  values of the  $(100)^+$  and  $(101)^+$  satellites. The intensities of the nuclear reflections and their satellites were then obtained from a  $\theta-2\theta$  scan. The intensity measurements were performed with two different detector configurations: one with no collimation between the sample and the 2-in.-diam  $\text{BF}_3$  detector and the other with a 10-min collimator in front of the detector. The latter configuration was used to resolve those satellites which were close to other reflections. The intensity ratios for the different reflections obtained with these two configurations were found to agree, to within experimental precision. In order to assess the presence of any hysteresis effects the intensities and the wave vector of the magnetic structure were measured on cooling as well as warming of the crystal. The intensities and wave vector were found to be reproducible, in the sense that repeated measurements on cooling (or warming) of the crystal agreed to within experimental precision. The magnetostriction effects,

in our sample, were studied by following the temperature variation of the  $a$  and  $c$ -axis lattice constants. The lattice constants were obtained by measuring the scattering angles of the  $(008)$  and  $(400)$  nuclear reflections.

In order to ascertain whether the observed satellites were due to (or contaminated by) simultaneous Bragg scattering, a Renninger-type<sup>10</sup> of experiment was performed. With the counter and crystal position optimized for the particular satellite, the crystal was rotated about the scattering vector. The possibility of the  $(000)^5$  and  $(000)^3$  satellites (observed between  $20^\circ\text{K}$  and  $50^\circ\text{K}$ ) being Renninger peaks was carefully examined. For each of these satellites the detector and crystal were optimized for Bragg reflection, and the crystal was rotated about the  $c$  axis. Because of the symmetry of the crystal a  $30^\circ$  rotation was sufficient. It was concluded that these satellites are not due to simultaneous Bragg scattering, since no variation in their intensity was observed upon rotation of the crystal. On the other hand, this type of experiment proved that the  $(001)$  "reflection" observed in the ferromagnetic spiral region was due to simultaneous Bragg scattering. The possibility of any satellites being due to the  $\frac{1}{2}\lambda$  contamination of the incident beam has been assessed by measurements with the incident neutron beam filtered by a Pu filter.

### III. EXPERIMENTAL RESULTS AND DISCUSSION

The observed integrated reflectivities of selected satellites and some nuclear reflections are plotted versus temperature in Figs. 1-3. In Fig. 4 the FWHM of the  $(101)^-$  and  $(002)^-$  reflections are plotted versus temperature in the vicinity of the Néel and the basal-plane-moment-ordering temperature.

#### A. Transition temperatures

At approximately  $84^\circ\text{K}$  the  $c$ -axis moment of Er orders in a sinusoidally modulated magnetic structure with wave vector parallel to the  $c$  axis (CAM), as evidenced by the observation of first-order magnetic satellites of all but the  $(00l)$  nuclear reflections (Fig. 1). Peaks at the positions of the first-order magnetic satellites were observable at temperatures as high as  $90^\circ\text{K}$ . However, the FWHM of these satellites was found to increase by approximately  $0.6^\circ$  above  $84^\circ\text{K}$  [Fig. 4(b)]. This observation indicates that the presence of the first-order satellites above  $84^\circ\text{K}$  is due to short-range order. The measured satellite intensities did not show, to within experimental precision, any significant hysteresis effects. The presence of short-range order and the absence of any hysteresis effects are consistent with a second-order transition in the vicinity of  $84^\circ\text{K}$ . Specific-heat

measurements<sup>5</sup> do indeed indicate that the transition is of the second order. A Néel point  $T_N$  of 84.4 °K was obtained by extrapolating the intensities of the first-order satellites from the temperature regime where no appreciable broadening was observed.

At approximately 52 °K the basal-plane moment orders in a spiral with wave vector parallel to the  $c$  axis, as evidenced by the appearance of first-order satellites of the  $(00l)$  nuclear reflections (Fig. 3). The presence of these first-order satellites at temperatures as high as 60 °K has been attributed to short-range order, since their FWHM was found to increase by approximately 0.7° above 52 °K [Fig. 4(a)]. The measured satellite intensities did not show any appreciable hysteresis effects in the vicinity of 52 °K. These observations are consistent with a second-order transition at this temperature. Specific-heat measurements<sup>5</sup> indicate that the transition is of the second order. A basal-plane-ordering temperature  $T_B$  of 52.4 °K was obtained by extrapolating the intensities of first-order satellites from the temperature regime where no appreciable broadening was observed.

Below a temperature  $T_C$  of approximately 18 °K an additional contribution to the intensity of all but the  $(00l)$  nuclear reflections has been observed. This implies ferromagnetic alignment of the  $c$ -axis moment. In the vicinity of this transition temperature the first-order satellite intensities exhibit a hysteresis of approximately 1.5 °K (Fig. 1). No short-range-order effects were observed in the vicinity of this transition temperature. These observations indicate that the transition at 18 °K is of the first order.

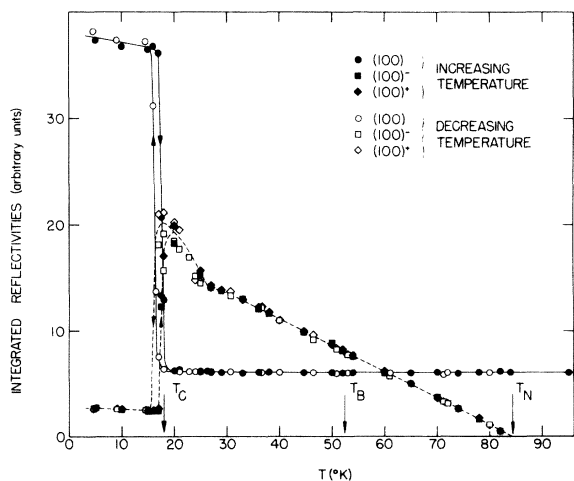


FIG. 1. Integrated reflectivities of the  $(100)$  nuclear reflection and its first-order satellites  $(100)^*$  vs temperature.

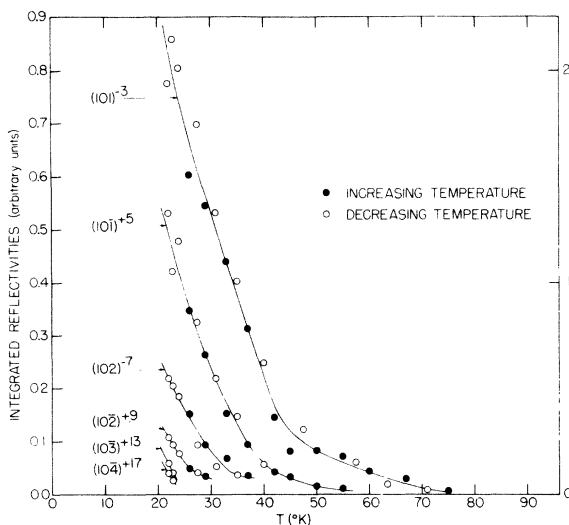


FIG. 2. Integrated reflectivities of the higher-order harmonics of the  $c$ -axis moment vs temperature. The third- and fifth-order harmonics are referred to the scale on the right-hand side of the graph. The seventh through the 17th harmonics are referred to the scale on the left-hand side of the graph.

### B. Magnetic structure

As the temperature is decreased below the Néel point, the CAM structure gradually deviates from a purely sinusoidal modulation, as evidenced by the appearance of higher-order satellites (Fig. 2). Higher-order satellites up to 17th order have been observed. The third- and fifth-order satellites were of measurable intensity at temperatures as high as 75 and 55 °K respectively. Two remarks should be made with regard to this observation. First, the higher-order harmonics appear before the first-order  $c$ -axis moment reaches its maximum value consistent with the crystal-field anisotropy. Second, the appearance of the higher-order harmonics is not connected in any way with the ordering of the basal-plane moment as might be inferred from previous measurements.<sup>1</sup> These results are in agreement with recent measurements by Atoji.<sup>11</sup>

Between 50 °K and 18 °K third- and fifth-order satellites of the  $(00l)$  nuclear reflections were observed (insert of Fig. 3). These higher-order harmonics were not seen in the original investigation<sup>1</sup>; however, they have also been observed in recent measurements by Atoji.<sup>11</sup> A systematic search for the seventh-order satellite, in the same temperature region, was inconclusive as a result of the higher background at the scattering angle of this satellite. [In this temperature region the seventh-order satellite is between the  $(002)^-$  and  $(002)^+$  reflections.] In addition, a careful search

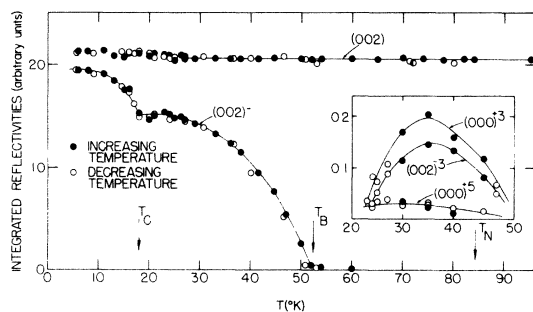


FIG. 3. Integrated reflectivities of the (002) and (002)<sup>-</sup> reflections vs temperature. The third and fifth harmonics of the basal-plane moment are plotted in the insert.

failed to reveal the presence of these higher-order satellites below 18 °K, the ferromagnetic transition temperature of the *c*-axis moment. This observation suggests coupling of the basal-plane moment to the *c*-axis modulated structure. It is well known that the basal-plane anisotropy would manifest itself by the appearance of fifth- and seventh-order satellites. On the other hand, the anisotropy of the magnetoelastic energy may introduce a third-order satellite. Thus the basal plane and the magnetoelastic anisotropy could be the origin of the higher-order basal-plane satellites observed in the present experiment. However, the anomalous temperature dependence of the basal-plane satellites, in particular their absence in the ferromagnetic spiral phase, awaits a detailed theoretical explanation.

### C. Temperature dependence of magnetic periodicity

The observed temperature dependence of the wave vector *q* of the periodic magnetic structure is given in Fig. 5. The wave vector, in units of 1/*c*, is 0.283 at 84 °K and increases to a value of

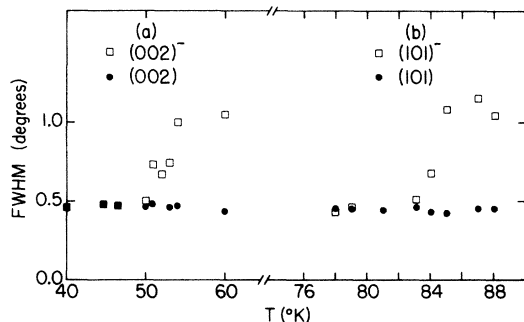


FIG. 4. (a) Full widths at half-maximum (FWHM) of the (002) and (002)<sup>-</sup> reflections in the vicinity of the basal-plane ordering temperature. (b) FWHM of the (101) and (101)<sup>-</sup> reflections in the vicinity of the Néel point.

0.291 at 52 °K. From 52 °K to 24 °K the wave vector decreases monotonically to a value of 0.250 and remains constant at this value down to approximately 18 °K. At this temperature the wave vector decreases to 0.238 and remains constant as the temperature is decreased to 6 °K. The measurements were performed during warming as well as cooling of the sample and significant hysteresis effects have been observed (Fig. 5). The results were reproducible, in the sense that the same *q* value was obtained after repeated warmings (or coolings) of the crystal. It should be pointed out that significant differences exist between the present data and those of Cable *et al.*,<sup>1</sup> in particular the hysteresis effects observed in the present experiment are less pronounced (Fig. 5). These differences are possibly due to the different purity of the samples. The temperature dependence of the magnetic periodicity, observed in the present experiment, does not agree with the Miwa-Yosida theory.<sup>12</sup> On the other hand, the data are in good agreement, in the (18–84) °K temperature region, with theoretical calculations<sup>13</sup> assuming a free-electron Fermi surface (Fig. 5). This observation implies that the distortion of the Fermi surface by the superzone boundaries, which result from the periodicity of the magnetic structure, is mainly responsible for the temperature dependence of the wave vector. At 18 °K Elliott and Wedgewood<sup>13</sup> predict a discontinuous change of the wave vector in a direction opposite to that found in our measurements (Fig. 5). In their model this discontinuous step is the net result of two opposite effects: (a) an increase in *q* due to the loss of the contribution of the *c*-axis modulated moment to the gap at the superzone boundaries; and (b) a decrease due to the ferromagnetic ordering which introduces new

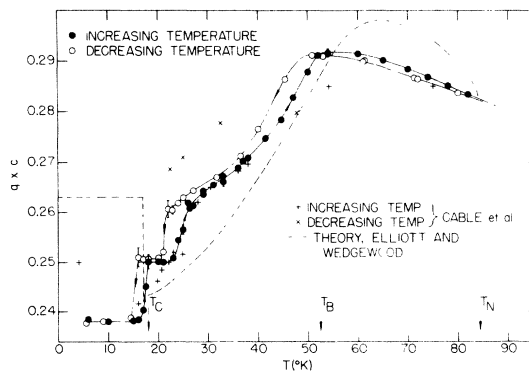


FIG. 5. Temperature dependence of the wave vector compared with the experimental results of Cable *et al.* (Ref. 1), and the theoretical calculation of Elliott and Wedgewood (Ref. 13). The theoretical curve has been normalized to our data at 84 °K.

gaps at the original Brillouin-zone boundaries. In addition, at 18 °K there is a substantial discontinuous increase in the magnetoelastic energy, not included in the theory, which will tend to decrease the magnitude of the wave vector. Our observations imply that the latter two effects are larger than the effect of the loss of the contribution to the gap at the superzone boundaries of the  $c$ -axis modulated moment. The measured temperature dependence of the wave vector shows an inflection point at approximately 33 °K possibly associated with a commensurate structure of 15 layers. At approximately 23 °K the magnetic structure becomes commensurate with an eight-layer period. These transitions are probably related to the  $c$ -axis susceptibility anomalies observed by Taylor *et al.*<sup>3</sup> and Spedding and Gray.<sup>2</sup> This may be seen from the following argument based on the molecular-field approximation. Consider a purely sinusoidal  $c$ -axis moment structure, and assume a weak-field  $\delta H$  applied along the  $c$  axis. The change in the  $c$  axis moment of the  $i$ th atom will be given by

$$\delta M_i = \left( \frac{g \mu_B J}{kT} \right)^2 B'_J \left( \frac{g \mu_B J H_i^M}{kT} \right) \delta H, \quad (1)$$

where  $H_i^M$  is the molecular field along the  $c$  axis and  $B'_J$  is the derivative of the Brillouin function. The  $c$ -axis susceptibility is then given by

$$\chi = \left( \frac{g \mu_B J}{kT} \right)^2 \sum_i B'_J \left( \frac{g \mu_B J H_0 \sin(\vec{q} \cdot \vec{R}_i)}{kT} \right), \quad (2)$$

where we have written the molecular field in a sinusoidal form. By the Bloch theorem, the sum in Eq. (2) will have a  $q$ -dependent contribution which will peak sharply when  $\vec{q}$  is a submultiple of a  $c$ -axis reciprocal-lattice vector.

#### D. Magnetostriction

The temperature variation of the lattice constants, determined from the measured (400) and (008) scattering angles, is given in Fig. 6. Below 52 °K, the basal-plane ordering temperature, the  $c$ -axis

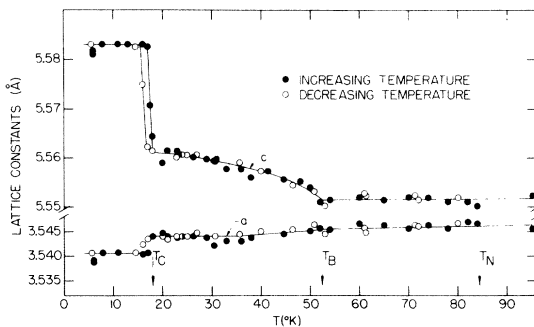


FIG. 6. Lattice constants  $c$  and  $a$  vs temperature.

lattice constant begins to expand with decreasing temperature. At 18 °K, the ferromagnetic transition temperature of the  $c$ -axis moment, there is a large discontinuous increase in the  $c$ -axis lattice-constant ( $\Delta c/c \approx 0.4\%$ ). All of the  $c$ -axis lattice-constant changes are reflected inversely in the  $a$ -axis lattice constant. These observations are in good agreement with x-ray<sup>14</sup> and magnetostriction measurements.<sup>15</sup>

#### E. Magnetic moments

The intensity measurements have been analyzed following the procedure outlined by Cable *et al.*<sup>1</sup> and Koehler.<sup>16</sup> For  $T > T_C$ , the  $c$ -axis moment  $[\mu_{||}(i)]$  and the basal-plane moment  $[\mu_{\perp}(i)]$  of the  $i$ th atom may be written as

$$\mu_{||}(i) = \sum_n \mu_{||}^{(n)} \cos[n(2\pi q z_i) + \alpha_n], \quad (3a)$$

$$\mu_{\perp}(i) = \sum_n \mu_{\perp}^{(n)} \cos[n(2\pi q z_i) + \beta_n], \quad (3b)$$

where  $n$  is an odd integer,  $z_i$  the position along the  $c$  axis of the  $i$ th atom in units of  $c$ ,  $q$  the magnitude of the wave vector in units of  $1/c$ , and  $\alpha_n, \beta_n$  are phase angles. It is easily shown that the Fourier coefficients in (1) can be expressed in terms of structure factor ratios by

$$\mu_{||}^{(n)} = \left[ \frac{1}{\sin^2 \Phi} \left( \frac{4b^2 (F_{(hkl)}^2)^{\pm n} / F_{(hkl)}^2}{P_0^2 f^2(\theta)} - (1 + \cos^2 \Phi) (\mu_{\perp}^{(n)})^2 \right) \right]^{1/2}, \quad (4a)$$

$$\mu_{\perp}^{(n)} = \left( \frac{4b^2 (F_{(00l)}^2)^{\pm n} / F_{(00l)}^2}{P_0^2 f^2(\theta) (1 + \cos^2 \Phi)} \right)^{1/2}, \quad (4b)$$

where  $F_{(hkl)}^{\pm n}, F_{(hkl)}$  are the  $n$ th-order magnetic-satellite and nuclear-structure factors, respectively,  $\Phi$  the angle between the scattering vector and the  $c$ -axis,  $b$  the coherent nuclear-scattering amplitude,  $f(\theta)$  the magnetic form factor, and  $P_0$  a numerical factor. With  $P_0^2 = 0.0725 \text{ cm}^2$  the Fourier coefficients in Eq. (4) are in units of Bohr magnetons.

For  $T < T_C$ , the magnetic structure of erbium is a simple ferromagnetic spiral with its screw axis along the  $c$ -axis of the crystal. In this case  $\mu_{\perp}$  can be obtained from Eq. (4b) and  $\mu_{||}$  is given by

$$\mu_{||} = \frac{b (F_{(hkl)} / F_{(hkl)_m})}{P_0 f(\theta) \sin \Phi}, \quad (5)$$

where  $F_{(hkl)_m}$  is the magnetic-structure factor of the  $(hkl)$  reflection.

The ratios of the magnetic to the nuclear-structure factors have been obtained from the ratios of the measured integrated reflectivities. We used an experimentally determined form factor obtained from the form-factor data of the present experiment,<sup>17</sup> those of Cable *et al.*,<sup>1</sup> and the small-angle-scattering data of Koehler and Wollan.<sup>11</sup> This

procedure has been adopted since a relativistic form-factor calculation is not presently available. In analyzing the data, a value  $b = 0.80 \times 10^{-12}$  cm was adopted<sup>18</sup> for the coherent nuclear-scattering amplitude of erbium. The results of the moment analysis are summarized in Fig. 7.

Throughout the ferromagnetic spiral region the total ordered moment per erbium atom is very close to its maximum value. At 6°K,  $\mu_{\parallel}$  and  $\mu_{\perp}$  are  $(7.80 \pm 0.12)\mu_B$  and  $(4.44 \pm 0.12)\mu_B$ , respectively, and within experimental precision the magnetic moment per atom reaches its maximum value of  $9.0\mu_B$ . At this temperature the cone angle is  $29.6^\circ$ , in excellent agreement with bulk magnetization measurements.<sup>2</sup>

At 22°K the first-order basal plane moment is  $3.8\mu_B$  and the first-order  $c$ -axis moment is  $10.5\mu_B$ . Thus the phases in Eq. (3a) must be such that the  $c$ -axis moment does not exceed approximately  $8.2\mu_B$ , since the maximum total moment per atom is  $9.0\mu_B$ . It is to be noted that if our measured  $c$ -axis Fourier amplitudes are combined with the choice of phases  $\alpha_n = n(\frac{5}{8}\pi)$ , postulated by Cable *et al.*,<sup>1</sup> the total moment on some erbium atoms would exceed  $9.0\mu_B$ . Although the detailed structure cannot be established (in the absence of a knowledge of the phases of the various harmonics), some insight into the general features of the magnetic structure may be obtained by examining the

root-mean-square  $c$ -axis moment given by

$$\langle \mu_{\parallel}^2 \rangle^{1/2} = \left( \frac{1}{2} \sum_n (\mu_{\parallel}^{(n)})^2 \right)^{1/2} . \quad (6)$$

This quantity was calculated from the amplitudes of the various harmonics and was found to increase smoothly with decreasing temperature. At 22°K, just above the temperature at which the structure locks into an eight-layer repeat arrangement, the root-mean-square  $c$ -axis moment is  $(7.7 \pm 0.2)\mu_B$  which is essentially the maximum value of the  $c$ -axis moment consistent with the crystal anisotropy. This implies that the magnetic structure approaches a configuration in which one-half of the atoms have their  $c$ -axis moments parallel and the other half antiparallel to the  $c$  axis, with every atom having a  $c$ -axis moment of approximately  $7.7\mu_B$ .

#### IV. SUMMARY

At 84.4°K the  $c$ -axis moment of erbium orders in a sinusoidally modulated magnetic structure, with wave vector along the  $c$  axis. Higher-order modulations along the  $c$  axis have been observed as the temperature was decreased below the Néel point. The third- and fifth-order  $c$ -axis harmonics were of measurable intensity at temperatures as high as 75°K and 55°K, respectively. Thus the  $c$ -axis structure deviates from a purely sinusoidal modulation before the first-order moment reaches the maximum value of the  $c$ -axis moment ( $7.8\mu_B$ ). Higher-order  $c$ -axis modulations up to the 17th order have been observed as the temperature was decreased down to 22°K.

At 52.4°K the basal-plane moment was found to order in a spiral with wave vector equal to that of the  $c$ -axis moment. Third- and fifth-order harmonics of the basal-plane moment were observed between 50°K and 18°K. The basal plane and the magnetoelastic anisotropy could be the origin of these higher-order harmonics of the basal-plane moment. At 22°K the first-order basal-plane moment is  $3.8\mu_B$  and the first-order  $c$ -axis moment is  $10.5\mu_B$ . Thus the phases of the various  $c$ -axis harmonics must be such that the  $c$ -axis moment does not exceed  $8.2\mu_B$ . It has been found that this condition cannot be satisfied by the simple choice of phases suggested by previous measurements.<sup>1,16</sup> At this temperature the root-mean-square average  $c$ -axis moment per erbium atom is  $7.7\mu_B$ , which is essentially the maximum  $c$ -axis moment consistent with the crystal anisotropy. This implies that the magnetic structure approaches a configuration in which one-half of the atoms have their  $c$ -axis moments parallel and the other half antiparallel to the  $c$  axis, with every atom having a  $c$ -axis moment of approximately  $7.7\mu_B$ .

Below 18°K the magnetic structure of erbium is a ferromagnetic spiral with its screw axis along

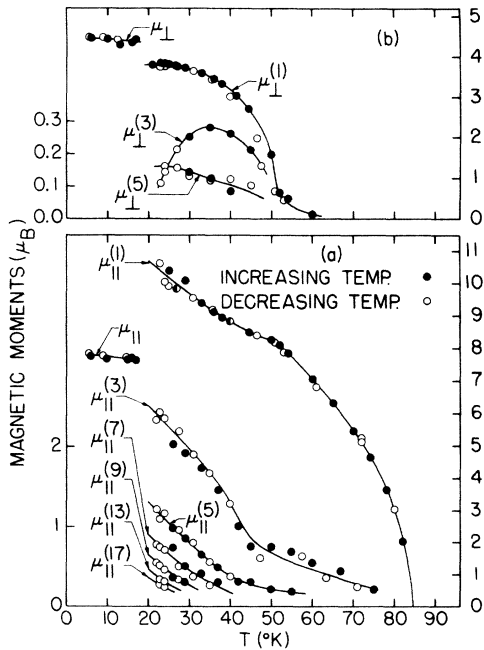


FIG. 7. Magnetic moments vs temperature: (a)  $c$ -axis moments, (b) basal-plane moments. The moments  $\mu_{\parallel}$ ,  $\mu_{\parallel}^{(1)}$ , and  $\mu_{\perp}$ , and  $\mu_{\perp}^{(1)}$  refer to the scale on the right-hand side of the graph.

the  $c$  axis of the crystal. At 6 °K,  $\mu_1$  and  $\mu_2$  have been found to be  $(7.80 \pm 0.12)\mu_B$  and  $(4.44 \pm 0.12)\mu_B$ , respectively, so that within experimental precision the magnetic moment per atom is the free-ion value of  $9.0\mu_B$ . The cone angle at this temperature is 29.6°.

First-order  $c$ -axis satellites were observed above the Néel point at temperatures as high as 90 °K. However, their FWHM increased dramatically above the Néel point. This observation indicates that the presence of the first-order  $c$ -axis satellites above the Néel point is due to short-range-order effects. Significant short-range-order effects were also observed above the basal-plane-moment ordering temperature. No significant hysteresis effects were observed in the vicinity of the Néel point and basal-plane-moment ordering temperature. The presence of short-range-order effects and the absence of any hysteresis effects are consistent with second-order transitions at these temperatures. The transition at 18 °K exhibits significant hysteresis effects, and no short-range-order effects were observed above this transition temperature. This indicates a transition of the first order in the vicinity of this temperature.

The temperature dependence of the wave vector

of the magnetic structure is in good agreement, in the (84–18) °K temperature region, with theoretical calculations by Elliot and Wedgewood.<sup>13</sup> This indicates that the main mechanism for the temperature dependence of the magnetic periodicity is the distortion of the Fermi surface by the superzone boundaries, introduced by the periodic magnetic ordering. At approximately 23 °K the magnetic structure becomes commensurate with an eight-layer period and at 33 °K an inflection point is observed, possibly associated with a commensurate structure of 15 layers. These transitions could be related to the susceptibility anomalies observed in the vicinity of these temperatures.

The temperature dependence of the  $a$ - and  $c$ -axis lattice constants was measured in the (84–6) °K temperature region. Below approximately 52 °K, the basal-plane-moment ordering temperature, significant magnetostriction effects were observed in quite good agreement with x-ray<sup>14</sup> and magnetostriction measurements.<sup>15</sup>

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<sup>17</sup>These results together with form-factor measurements by polarized neutron techniques (presently in progress) will be published elsewhere.

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