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Nuclear Hyperfine Structure in Er^{166}†

R. L. COHEN AND J. H. WERNICK
Bell Telephone Laboratories, Murray Hill, New Jersey

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The Mössbauer effect has been used to study hyperfine structure in the 81-keV ($2^+ \rightarrow 0^+$) transition in Er^{166}, using $HoAl_2$ as a source. Absorbers of Fe_2Er, Er metal, $ErFe_3Mn$, and Er_2O_3 were studied with the following results: Magnetic moment of the excited state, 0.61 nm; quadrupole moment, approximately -1.6 b; magnetic moment of the Er^{3+} ion in erbium metal at 21°K, 7.5 ± 0.6 μ_B. The nuclear moments are in good agreement with the values predicted from the collective model, and with other experimental determinations. The resonance absorption is much less than 1%, but the relatively large hyperfine interaction and high counting rates possible make the measurements fairly easy.

STUDIES of nuclear hyperfine structure in rare-earth (RE) isotopes are interesting because of the information that can be gained about nuclear moments in the deformed region and electronic structures of RE ions in solids. The Mössbauer effect can be used to study nuclear hyperfine interactions in a number of RE isotopes, but there have been two problems restricting the application of this technique: the problem of obtaining a monochromatic source to facilitate studies of absorber hyperfine structure, and the problem of "calibrating" the hyperfine interactions by measurements on an absorber material in which the electronic wave functions are well known. The present work describes a solution to these problems for the isotope Er^{166}; the possible extension of these techniques to other heavy rare-earth isotopes is obvious.

The series of cubic Laves-phase[1] intermetallic compounds should form a suitable surrounding for RE sources, since the high symmetry of the RE site surrounding eliminates quadrupole splitting from the crystal field, and some of the systems are paramagnetic even at low temperatures, so that there is no net magnetic hyperfine interaction.

We have taken advantage of this in the current experiments by using the intermetallic $HoAl_2$[1,2] as a source. $HoAl_2$ was neutron irradiated to produce the 27-h Ho^{166}, which beta decays to the 81-keV level in Er^{166}.[3] The source was used successfully without annealing; apparently, the radiation damage effects are small and could possibly be annealed out at room temperature. The linewidth obtained was 2–3 times broader than that to be expected from lifetime considerations,[4] but nevertheless much less than the magnetic hyperfine interactions observed. The source temperature was approximately 25°K in all of these experiments.

The experimental arrangement used transmission geometry, with parabolic motion applied to the source with a drive which has already been described.[5] The gamma rays passing through the absorber were detected by a scintillation detector, and data were stored in a 400-channel analyzer used in the time mode. Counting rates as high as 20 000 counts/sec were obtained.

The absorber compounds studied were Fe_2Er, Er metal, Fe_3MnEr, and Er_2O_3. All the measurements were made at 21°K, where the first three compounds are magnetically ordered.

THE NUCLEAR HYPERFINE INTERACTION

The nuclear hyperfine interaction results from the interaction of the nuclear moments, μ and Q,[6] with the internal fields, and can be written

$$E=E_m+E_Q=\mu H_{\text{int}}(m/I) +eQV_{zz}[3m_I^2-I(I+1)]/[4I(2I-1)], \quad (1)$$

where E_m and E_Q are the magnetic and electric interaction energies, respectively, H_{int} is the internal magnetic field and V_{zz} is the electric field gradient, assumed axially symmetric at the nucleus. The nuclear ground state ($I=0$) is not split; the 2^+ excited state is split into five equally spaced levels by the magnetic interaction, and these levels are further shifted by the quadrupole interaction. The resulting hyperfine structure of the 81-keV transition is shown in Fig. 1. In absorption, five lines of equal strength are expected.

No appreciable isomer shifts were observed in the present experiments; this is not surprising since the nuclear size change should be very small for rotational states.

RESULTS FROM Fe_2Er

The compound Fe_2Er is a cubic Laves-phase intermetallic with properties which facilitate the interpretation of hyperfine-interaction data. These properties have been discussed in detail elsewhere[7] for the similar compound Fe_2Tm, and we simply assert here that in Fe_2Er, at low temperature, the Er ions are magnetized

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† A preliminary report of this work was presented at the Third International Mössbauer Conference [Rev. Mod. Phys. **36**, 393 (1964)].

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[6] Throughout this paper, Q indicates the spectroscopic quadrupole moment.

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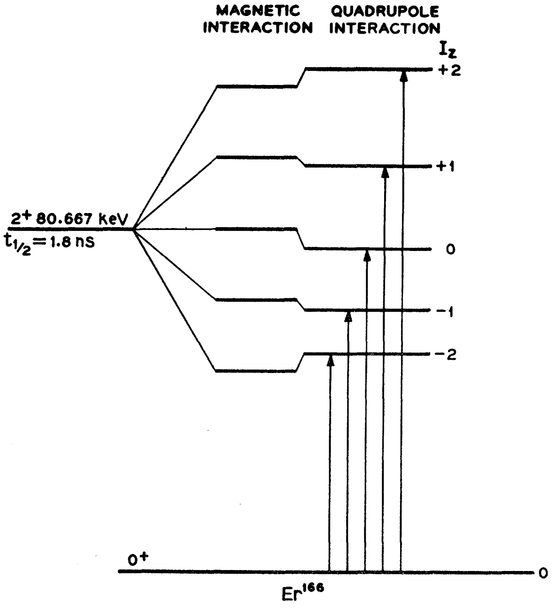

FIG. 1. Hyperfine structure of the 81-keV transition in Er^{166}.

to the gJ value through the exchange interaction with the iron sublattice; that crystal field effects are weak, and that we can consider the fields producing the nuclear hyperfine interaction as originating entirely in the partly filled $4f$ electron shell. Under these assumptions, from Refs. 7 and 8, we get the following formula for the internal fields:

$$H_{\text{int}}=2\mu_B\zeta\langle r^{-3}\rangle_{\text{eff}}J \tag{2a}$$

$$V_{zz}=e\beta\langle r^{-3}\rangle_{\text{eff}}[3J^2-J(J+1)](1-R). \tag{2b}$$

In these formulas, $\zeta=176/425$, $\beta=-4/2975$, and $\langle r^{-3}\rangle_{\text{eff}}$ are matrix elements for the $^4I_{15/2}$ $4f$ shell of the Er^{3+} ion.

The use of the term $\langle r^{-3}\rangle_{\text{eff}}$ rather than $\langle r^{-3}\rangle$ is intended to show that there may be some magnetic shielding effects due to closed-shell distortions, and that these may make the "effective" $\langle r^{-3}\rangle$ different from the Coulombic $\langle r^{-3}\rangle$ calculated for the $4f$ electrons. The factor $(1-R)$ then represents the difference between the effects of magnetic and electric shielding of the $4f$ electrons; this differs slightly from the conventional usage.

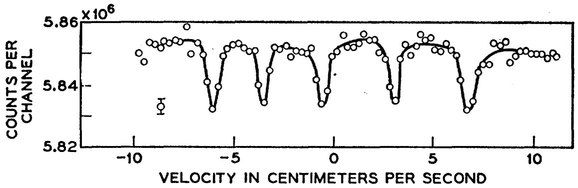

FIG. 2. Resonance absorption pattern of Er^{166} in Fe_2Er at 20°K.

This point is discussed in greater detail in Ref. 9. In most previous work with RE hyperfine structure and g-factor measurements, the calculated Coulombic $\langle r^{-3}\rangle$ values have been used to evaluate the internal fields. This technique not only completely disregards any magnetic shielding effects, but is subject to considerable uncertainty because the calculated values of $\langle r^{-3}\rangle$ vary widely (see Refs. 10 and 11 and references therein). In the present experiment, the internal field is evaluated using a value of $\langle r^{-3}\rangle_{\text{eff}}$ obtained by extrapolation from experiments with Tm^{169} in Fe_2Tm[7]; since Tm ($Z=69$) is similar to Er ($Z=68$), this process should be extremely accurate and should be essentially independent of any shielding effects. A somewhat similar technique was used by Gerdau *et al.*[11] in the analysis of angular correlation results.

The five-line resonance absorption pattern obtained in Fe_2Er at 20°K is shown in Fig. 2. Using the value of $\langle r^{-3}\rangle_{\text{eff}}=11.5$ au obtained by the extrapolation from Tm^{169}, the internal field can be calculated to be 8.4×10^6 Oe from Eq. (2a), and the magnetic moment of the 2^+ state is then (±)0.61±0.03 nm. Table I shows[12,13] the comparison of this value with other results. The agreement is seen to be excellent.

TABLE I. Magnetic moment values for the 81-keV state of Er^{166}.

Method	Value (nm)	$\langle r^{-3}\rangle$ used (a.u.)
Mössbauer effect[a]	±0.61 ±0.03	11.5
Collective-model calculation[b]	0.63	...
Angular correlation[c]	0.52 ±0.068	12.7
Angular correlation[d]	0.64 ±0.04	10.3
Angular correlation[e]	0.612±0.072	10.9
Mössbauer effect[f]	0.62 ±0.06	10.7

[a] Present result.
[b] Ref. 12, p. 48.
[c] Ref. 13.
[d] Ref. 13, recalculated in Ref. 12, p. 48.
[e] Ref. 13, recalculated in Ref. 11.
[f] Ref. 2.

From the positions of the five lines shown in Fig. 2 and Eqs. (1) and (2b), the quantity $(1-R)Q$ can be evaluated as -1.60 ± 0.16 b.[14] Magnetic shielding corrections (which produce the difference between $\langle r^{-3}\rangle_{\text{eff}}$ and $\langle r^{-3}\rangle_{\text{Coul}}$ are not accurately known, but are believed to be small relative to the electric shielding terms.[15] If we make the approximation that R arises

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entirely from electric shielding effects, we can use results in Tm^{169} [7,16,17] [where $(1-R)Q=-1.1$ b and $Q_{\text{theor}}(\delta=0.28)$ is -1.4 b] to calculate $(1-R)=0.78$. If we do the same calculation for the Er^{166} results, using $Q_{\text{theor}}=-2.1$ b $(\delta=0.28)$, we find $(1-R)=0.76$. The conclusion is either that $R\approx 0.23$, in approximate agreement with theoretical calculations, or that there is a systematic difference between measured nuclear quadrupole moments and those calculated from the collective model.

The present experiment incidentally shows that the magnetic hyperfine interaction is much larger than the electric interaction, confirming the validity of the analysis of the angular correlation data of Bodenstedt *et al.*[11,13]

RESULTS IN Er METAL AND Fe_3MnEr

Both of these materials showed, at 21°K, a five-line hyperfine structure characteristic of a magnetically ordered material. The values obtained for the ion moments were $7.5\pm0.6\,\mu_B$ in Er metal and $8.2\pm0.6\,\mu_B$ in Fe_3MnEr, assuming that the gJ value of $9\,\mu_B$ is obtained in Fe_2Er, and that the ion moment is proportional to the internal field. The value of the magnetization obtained in Er metal is consistent with the results of neutron diffraction measurements.[18] There was some indication in the Er metal spectrum that there might be a small range of moments for the Er ions; this would not be surprising considering the complex magnetic structure[18] of Er metal above 20°K.

RESULTS IN Er_2O_3

The interpretation of the absorption spectrum of Er_2O_3 tends to be relatively complicated because there are two inequivalent Er sites in a 3:1 population ratio. The spectrum obtained in the present experiment, shown in Fig. 3, is not directly comparable with the earlier results of Stanek,[19] since that work used Ho_2O_3 sources, which were not monochromatic at 20°K. Stanek obtained an extremely complicated spectrum which was attributed to 25 lines having the natural linewidth and 75 weaker lines forming a broad background; electric and magnetic hyperfine splittings were evaluated on this assumption. The splittings obtained by Stanek would lead us to expect five lines of equal intensity at approximately -3.6, -2.4, -0.6, 1.8, and 4.8 cm/sec for the site with population 3. This is clearly not observed in Fig. 3. Since there is no other evidence for magnetic ordering in Er_2O_3, one would expect the broad line obtained in the present work to be an unresolved combination of six lines (three from each of the two sites) resulting from quadrupole splitting of the excited state; no attempt was made, using this assumption, to decompose the pattern obtained.

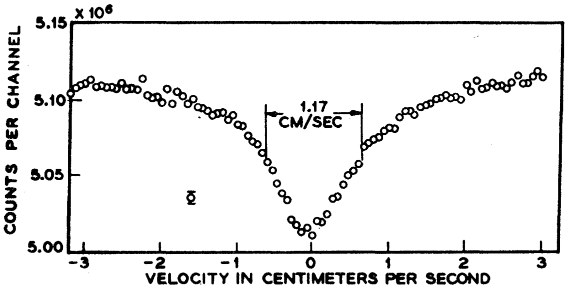

FIG. 3. Resonance absorption in Er_2O_3 at 20°K.

SUMMARY

In this paper the results of hyperfine structure measurements on Er^{166} have been presented. Through the analysis of these results, the nuclear magnetic moment of Er^{166} has been accurately determined, and information about the nuclear quadrupole moment and electric shielding factors has been obtained. The moments of the Er ions in two magnetically ordered compounds have been measured. These results are all in good agreement with theoretical calculations and with other experimental determinations.

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