Theoretical explanation of the Er C_{33}-versus-temperature curve in the ordered phase near T_N

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(Received 26 January 1982)

We have developed a general algorithm in order to study many static and dynamic magnetoelastic properties of a rare-earth metal, with the use of a general Hamiltonian already known in literature. As a specific application of our method we calculate the magnetic contribution to the Er C_{33} elastic constant in the region of ordered phase near T_N. In order to study the magnetic ordered phase we have adapted a method developed by Nagamiya.

I. INTRODUCTION

We have used the known theories of magnetostriction already developed by Callen and Callen[1,2] and Southern and Goodings.[3] In order to compare our results with experiment, we have considered a very detailed computer program. Our initial aim is to study as many magnetoelastic properties of the rare-earth metal as possible.

In this report we consider the behavior of the Er C_{33} elastic-constant—versus—temperature curve in the ordered phase near the Néel temperature. In order to study this behavior in this region we have made use of a generalization of Nagamiya's study on helical spin ordering.[4]

II. THE HAMILTONIAN

Assuming the equivalence of all ions in the crystal we adopt the general Hamiltonian

$$H=H_{\rm ex}+H_z+H_c+H_{\rm me}^{\rm I}+H_{\rm me}^{\rm II}+H_e \ . \tag{2.1}$$

In order to deal with the Heisenberg Hamiltonian $H_{\rm ex}$, we make use of the Weiss molecular-field hypothesis. In this way we may write

$$H_{\rm ex}=g\mu_B\Gamma M_0\vec{\sigma}\cdot\vec{J} \ , \tag{2.2}$$

where g is the Landé factor, μ_B the Bohr magneton, Γ is the Weiss constant, M_0 is the saturation magnetization, $\vec{\sigma}$ is the reduced magnetization ($\vec{\sigma}=\vec{M}/M_0$), and $\vec{J}$ is the total angular momentum operator. The Zeeman Hamiltonian is

$$H_z=g\mu_B\vec{J}\cdot\vec{H} \ , \tag{2.3}$$

where $\vec{H}$ is the external magnetic field. H_c in Eq. (2.1) is the crystal-field anisotropy energy. This Hamiltonian characterizes the electrostatic interaction of the $4f$ shell distribution of one ion with the (electric) crystal field formed by all other ions in the crystal. For this part of the Hamiltonian one may write

$$H_c=P_2^0Q_2^0(\vec{J})+P_4^0Q_4^0(\vec{J})+P_6^0Q_6^0(\vec{J})+P_6^6Q_{66}^+(\vec{J}) \ . \tag{2.4}$$

Q_l^m are the reducible tensor operators, P_l^m are the phenomenological crystal-field constants, the terms in P_2^0, P_4^0, and P_6^0 correspond to a uniaxial anisotropy, and P_6^6 means a basal anisotropy.

For the present purpose we consider the magnetoelastic Hamiltonian corresponding to one ion interaction $H_{\rm me}^{\rm I}$, including terms with $l=2$ only. This Hamiltonian may be written as

$$H_{\rm me}^{\rm I}=-(B_1^{\alpha,2}e_1^\alpha+B_2^{\alpha,2}e_2^\alpha)Q_2^0(\vec{J})-B^{\gamma,2}[e_1^\gamma Q_{22}^+(\vec{J})+e_2^\gamma Q_{22}^-(\vec{J})]-B^{\epsilon,2}[e_1^\epsilon Q_{21}^-(\vec{J})+e_2^\epsilon Q_{21}^+(\vec{J})] \tag{2.5}$$

$B_i^{\Gamma,j}$ are the phenomenological magnetoelastic coupling constants and e_i^Γ are the strains. The magnetoelastic Hamiltonian corresponding to the two-ion interaction $H_{\rm me}^{\rm II}$ is written as

$$H_{\rm me}^{\rm II}=J(G_1^{\alpha,0}e_1^\alpha+G_2^{\alpha,0}e_2^\alpha)\vec{\sigma}\cdot\vec{J}+J(G_1^{\alpha,2}e_1^\alpha+G_2^{\alpha,2}e_2^\alpha)(3\sigma_zJ_z-\vec{\sigma}\cdot\vec{J})+JG^{\gamma,2}[e_1^\gamma(J_x\sigma_x-J_y\sigma_y)+e_2^\gamma(J_x\sigma_y+J_y\sigma_x)]+JG^{\epsilon,2}[e_1^\epsilon(J_y\sigma_z+J_z\sigma_y)+e_2^\epsilon(J_x\sigma_z+J_z\sigma_x)] \ . \tag{2.6}$$

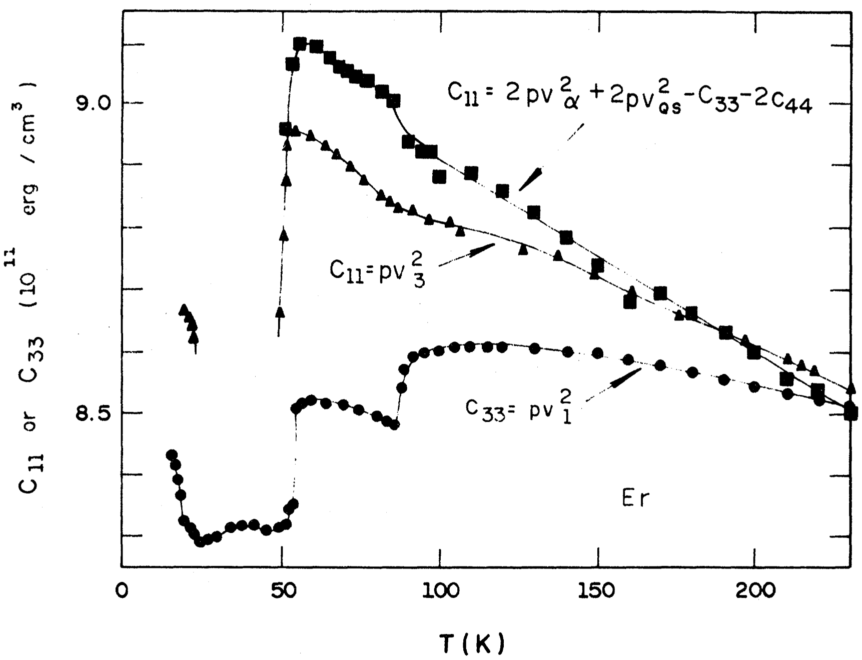

FIG. 1. Temperature dependence of two elastic constants for Er (Ref. 5).

$G_i^{\Gamma,j}$ are the phenomenological two-ion magnetoelastic coupling constants.

Finally, H_e in Eq. (2.1) is the Hamiltonian which represents the static interaction. We may write

$$H_e = \tfrac{1}{2}C_{11}^\alpha(e_1^\alpha)^2 + C_{12}^\alpha e_1^\alpha e_2^\alpha + \tfrac{1}{2}C_{22}^\alpha(e_2^\alpha)^2 + \tfrac{1}{2}C^\gamma[(e_1^\gamma)^2+(e_2^\gamma)^2] + \tfrac{1}{2}C^\epsilon[(e_1^\epsilon)^2+(e_2^\epsilon)^2] \;. \tag{2.7}$$

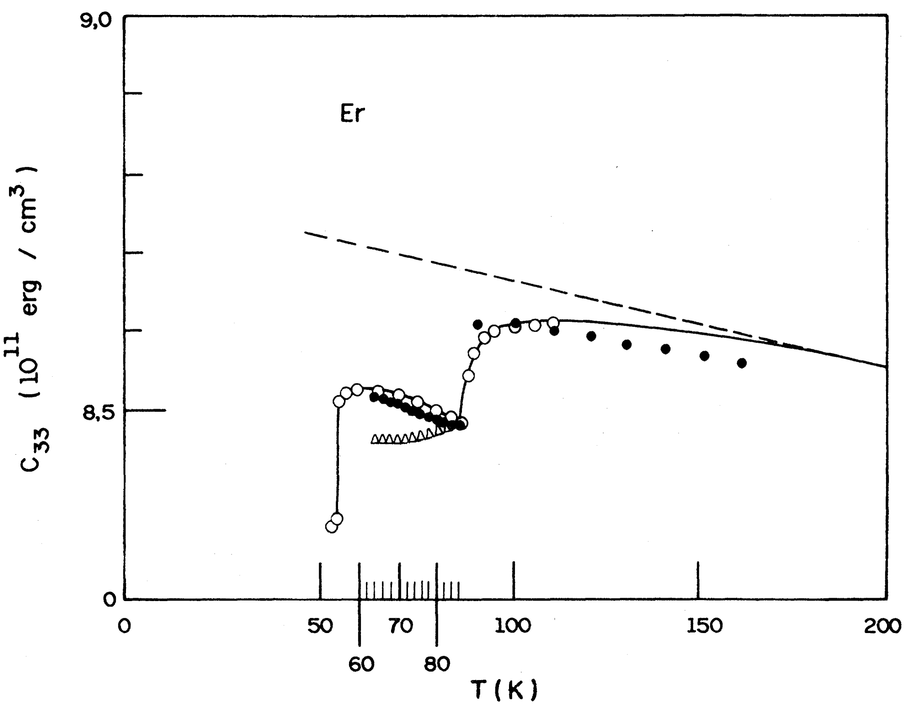

FIG. 2. Theoretical determination of the temperature dependence of C_{33} for Er in the neighborhood of ordered phase near T_N and in the paramagnetic region. Open circles are experimental values of Ref. 5. Open triangles and solid circles are two sets of values for different values of magnetostriction coefficients.

C_{ij}^{Γ} are the elastic constants. As we are interested in the magnetic contributions to the elastic constants, we use the relations

$$\Delta C_{ij}=\frac{\partial^2 U(\vec{\mathrm{H}})}{\partial e_i \partial e_j}-\frac{\partial^2 U(\vec{\mathrm{H}}=0)}{\partial e_i \partial e_j}\ , \qquad (2.8)$$

where $\vec{\mathrm{H}}$ is the external magnetic field. U is the free energy calculated through our computer program using the definition equation

$$U=\frac{\sum_n E_n \exp\left[-\frac{E_n}{T}\right]}{\sum_n \exp\left[-\frac{E_n}{T}\right]}\ , \qquad (2.9)$$

where E_n are the eigenvalues of the Hamiltonian operator obtained through a diagonalization in our computer program.

III. COMPARISON WITH EXPERIMENT

The behavior of the rare-earth metal elastic constants changes characteristically in a magnetic phase transition. In this report we have limited ourselves to the study of the C_{33} Er elastic constant in the neighborhood of the Néel temperature. In Fig. 1 the experimental curve of C_{33} versus temperature is shown.[5] Including some modification in our Hamiltonian in order to adopt part of the formalism discussed by Nagamiya,[4] we have obtained a very good concordance with experimental results. To our knowledge this is the first time that a comparison has been made between the experiment and a detailed calculation using a theoretical model which describes a magnetostriction property of a rare-earth metal in a magnetic-ordered-phase region.

Unfortunately, we do not yet have a good experimental set of values for all parameters appearing in the Hamiltonian. For this reason we must give a value for many of these parameters. We have considered the anisotropy constants (in K/ion) $P_2^0=-3.12\times10^{-1}$, $P_4^0=2.734\times10^{-4}$, $P_6^0=7.572\times10^{-7}$, and $P_6^6=-1.7\times10^{-6}$. For the magnetostriction coefficients we initially used the values $B_1^{\alpha}=2.4$, $B_2^{\alpha}=2.4$, $B^{\gamma}=-6.7$, $B^{\epsilon}=7.0$, $G_1^{\alpha,0}=0$, $G_2^{\alpha,0}=0$, $G_1^{\alpha,2}=0$, and $G_2^{\alpha,2}=0$. Our results are plotted in Fig. 2 with the points in open triangles. It is possible to obtain a better result if we consider all values stated above but $G_1^{\alpha,0}=-5$ and $G_2^{\alpha,0}=-3.5$. These points are plotted again in Fig. 2 as solid circles.

IV. CONCLUSION

As we have stated above, we have used Nagamiya's work in order to study the behavior of Er C_{33} elastic constant in the neighborhood of the Néel temperature. We have not applied our procedure in other regions of the ordered magnetic phase because we have not yet a treatment like that of Nagamiya for other values of the temperature in the ordered-phase region.

ACKNOWLEDGMENT

I would like to thank Professor P. L. Donoho from Rice University who suggested this problem to me and helped me in many instances.

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