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[15]Which fact may be taken as an indication that fluctuations in the data due to the proximity of the critical point are insignificant.

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Effects of Hydrostatic Pressure on the Magnetic Ordering of Heavy Rare Earths*

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The effects of hydrostatic pressure on the magnetic ordering of heavy rare earths are studied through the pressure shift of the electronic energy bands and the effects of this pressure shift on the indirect exchange. It is shown that the change in the ordering temperature of Gd, Tb, and Dy and the variation of the helical turn angle of Tb can be explained in this manner.

Many experiments have been performed to study the effects of hydrostatic pressure on the magnetic ordering of heavy rare earths.[1-6] Below a certain critical pressure where a crystallographic transition takes place, the magnetic ordering temperature of Gd, Tb, Dy, and Ho was found to decrease linearly with pressure by the order -1 K/kbar. The type of initial magnetic ordering is unchanged by pressure, i.e., just below the ordering temperature Gd is ferromagnetic while Tb, Dy, and Ho are antiferromagnetic.[4,6] However, neutron diffraction experiments have revealed a reduction of helical turn angle in Tb and Ho when pressure is applied.[6] The purpose of our work is to explain these results from the point of view that the magnetic ordering of these metals is to a large extent determined by their electronic energy bands and Fermi-surface geometry.[7-9] It will be shown that this approach does give a quantitative understanding of the observed effects.

The program of our study proceeds by first calculating the electronic energy bands of the metal under study, then computing the generalized susceptibility function $\chi(\vec{q})$ for a $\vec{q}$ vector along the c axis, and finally correlating the location and the size of the peak of $\chi(\vec{q})$ with the magnetic ordering properties. This is done for Gd, Tb, and Dy under 0 and 20 kbar of pressure. The pressure effects are deduced from the shift of the $\chi(\vec{q})$ curve. In the following paragraph we explain briefly these calculations.

We used the relativistic augmented-plane-wave (RAPW) method for the energy band calculation,[10] the details of which are given in Ref. 7. The crystal potential was approximated by a muffin-tin potential constructed from a superposition of atomic potentials including the full Slater exchange. The lattice parameters under pressure were deduced from the elastic constants of Gd,[11] Tb,[12] and Dy.[13,14] Their actual values are listed in Table I. The radius of the augmented-plane-wave (APW) sphere was chosen as 3.32 a.u. for Gd and as 3.16 a.u. for Tb and Dy. The same APW sphere radius was used for both the zero-pressure and the 20-kbar calculations. We selected a set of 32 plane waves as the basis functions so that the band calculation was convergent to within 0.002 Ry. Energy eigenvalues were calculated over a mesh of 147 points in 1/24th zone. The spline interpolation method was used to interpolate the bands over a mesh of 450 000 points in the full zone. The susceptibility calculation was fully described in Ref. 9. With the interpolated bands, we calculated $\chi(\vec{q})$ for $\vec{q}$ along $\Gamma A \Gamma$ in the double zone scheme over a

TABLE I. Lattice parameters of Gd, Tb, and Dy under 0- and 20- kbar hydrostatic pressure.

	Gd		Tb		Dy	
Pressure (kbar)	0	20	0	20	0	20
a(a.u.)	6.867	6.745	6.811	6.694	6.784	6.676
c(a.u.)	10.925	10.737	10.768	10.591	10.673	10.502

mesh of 60 points.

It seems appropriate at this point to discuss the limitations of this calculation. (a) The band calculation involves a whole series of approximations. There is no way to assess the accuracy of the result because of the lack of experimental Fermi-surface data. We took great care to do the zero-pressure and 20-kbar calculations in an identical manner in order to minimize random error. Also, by choosing a high enough pressure we hoped that the pressure shift would be large enough to be detectable above the noise level. (b) The $\chi(\vec{q})$ calculation has a 3% noise content. This is not a serious problem because the peak in $\chi(\vec{q})$ is usually broad enough so that the maximum can be picked out with little difficulty. (c) The susceptibility calculation is done with the paramagnetic band, so the conclusions apply only to the initial ordering properties. However, in reality the turn angle must be measured when there is a substantial amount of ordered moment. There is reasonable ground for comparing the theory with the experiment in case of Dy where the magnetoelastic effect is weak over most of the helical-ordering temperature range, but not so for Tb where we expect an important influence of magnetoelastic

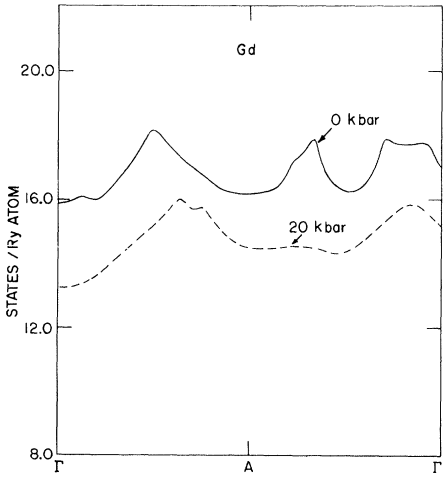

FIG. 1. Generalized susceptibility function for gadolinium in ΓAΓ direction at 0 and 20 kbar of hydrostatic pressure.

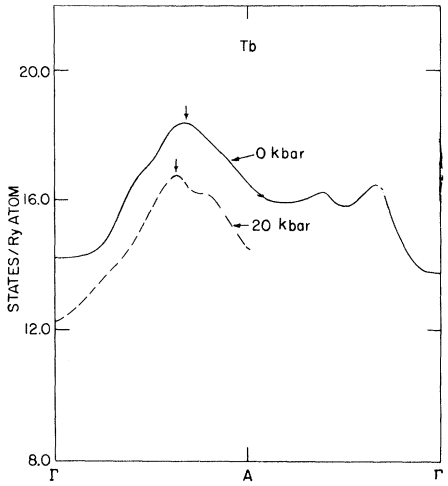

FIG. 2. Generalized susceptibility function for terbium in ΓAΓ direction at 0 and 20 kbar of hydrostatic pressure.

energy on the turn angle.[9] (d) The s-f matrix element is assumed to be pressure independent purely because of our great ignorance about this quantity.

The results of this investigation are summarized in Figs. 1–3 and in Table II. In the figures we plot the susceptibility function per spin per atom along the ΓAΓ direction. From Figs. 2 and 3 one can see the peaks of $\chi(\vec{q})$ for Tb and Dy shift to smaller q values when the pressure is applied and the sizes of the peaks are reduced. There is a small peak in the susceptibility function for Gd, but one should not take it seriously because it is probably wiped out by a q-dependent s-f matrix element. The shift in T_c or T_N is obtained from

$$T_c(P)/T_c(0) = \chi_0(P)/\chi_0(0)$$

for Gd, and

$$T_N(P)/T_N(0) = \chi_{max}(P)/\chi_{max}(0)$$

for Tb and Dy.[15] Here χ_{max} is the size of the peak of $\chi(\vec{q})$, and χ_0 is the static susceptibility. Table II displays the numerical results alongside the experimental values. The range of the measured values is given in case there is slight disagreement among the various investigators. In view of all the uncertainties in the calculation, the agreement with the experimental values must be termed

TABLE II. Dependence of ordering temperature and turn angle of heavy rare earths on hydrostatic pressure.

	Gd		Tb		Dy	
	Expt	Calc	Expt	Calc	Expt	Calc
dT/dP (K/kbar)	−1.56	−2.3	−0.8	−1.0	−0.4	−0.4
			~−1.1		~−0.6	
$d\omega/dP$ (°/kbar)	···	···	−0.36	−0.23	?	−0.38

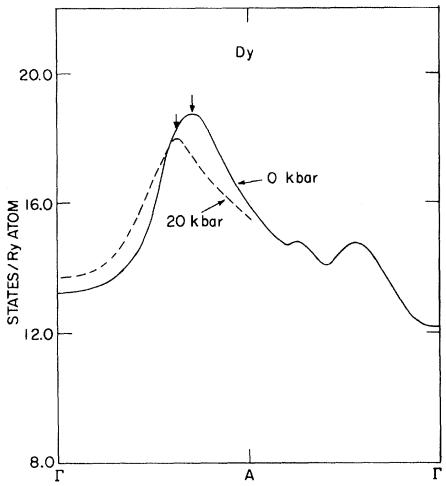

FIG. 3. Generalized susceptibility function for dysprosium in ΓAΓ direction at 0 and 20 kbar of hydrostatic pressure.

highly satisfactory. The energy bands and the density of states under pressure are not plotted because they closely resemble their zero-pressure counterparts.

In conclusion, we feel that the pressure dependence of the magnetic ordering of heavy rare earths can be explained on the basis of the pressure shift of the energy bands. Conversely, the good results of the present calculation lend further support to the contention that the initial magnetic ordering in these metals is mainly determined by the energy band structure through the indirect exchange mechanism.

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