we shall describe in the future.

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Scattering of Conduction Electrons by Magnetic Excitons in a Singlet Ground State System

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The electrical resistivity of $Tb_cY_{1-c}Sb$ has been measured as a function of temperature and of Tb concentration. The resistivity contribution from scattering of conduction electrons by Tb $4f$ electrons has been calculated in the paramagnetic regime in order to examine the competing effects of the crystal field and the exchange interaction. Excellent agreement with experiment is obtained for the entire range of c with one value for each of the two adjustable parameters, the Fermi momentum, and the electron-ion exchange constant.

Rare-earth metals and compounds normally undergo a magnetic phase transition due to the indirect exchange interaction between the magnetic $4f$ electrons. If the rare-earth ion is of the non-Kramers type, the crystal field may split the $4f$ multiplet in such a way that the lowest level is a singlet. Depending on whether the ratio of exchange to crystal field is larger or smaller than a critical value, the crystal will or will not order at the lowest temperatures.[1] The $Tb_cY_{1-c}Sb$ system is of particular interest since the exchange interaction between the Tb ions varies with c whereas the crystal field is virtually unaffected, thus allowing the behavior to be studied as the ratio passes through its critical value.[2] In this Letter we calculate the effect of the coexist-ence of magnetic exchange and crystal field on the resistivity in the paramagnetic temperature regime and compare this to our measured resistivity.

We have measured the resistivity of fifteen 2–6-mm-long single crystals of $Tb_cY_{1-c}Sb$ with various values of the Tb concentration in the temperature range from 1.5 to 300 K. The resistivity was determined by a four-terminal dc method and the temperature measured with a thermocouple.

Figure 1 shows the experimental results in the temperature range up to 30 K. The residual resistivity has been subtracted and each resistivity versus temperature curve has an arbitrary origin. Since the absolute resistivity for some of
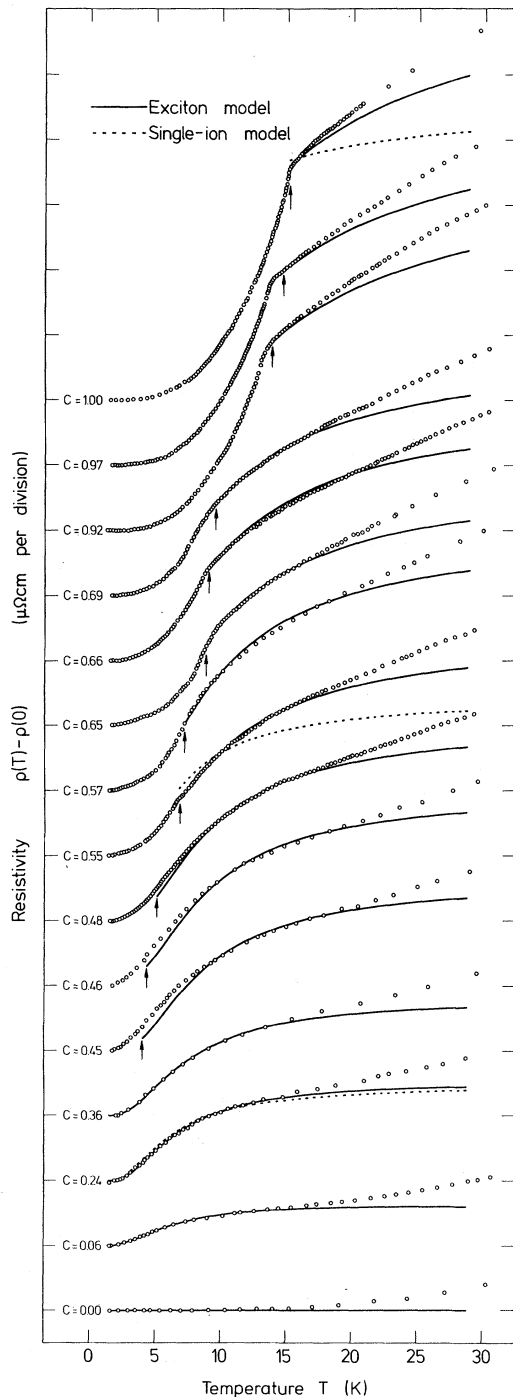
FIG. 1. Electrical resistivity of $Tb_cY_{1-c}Sb$. For each value of c the residual resistivity has been subtracted and the origin has been displaced. The arrows indicate the molecular-field transition temperature T_N. Above T_N the resistivity calculated from Eq. (1) is shown as a solid line. For comparison the single-ion model is shown for three values of c.

the very small samples was rather poorly defined, the resistivities have been adjusted such that all curves have the same high-temperature slope. The Tb concentration indicated in Fig. 1 was determined by neutron activation analysis giving an uncertainty of 0.02 in c. These values of c differ significantly (up to a difference in c of 0.14) from the nominal ones. These deviations we believe are due to segregation processes during the growth of the crystals. Electron-microprobe analyses did not, however, reveal any concentration gradients in the single crystals.

As a consequence of the exchange interaction between the conduction electrons and the unfilled Tb $4f$ shell ($J = 6$) a temperature-dependent (magnetic) resistivity contribution can be observed. The gradual increase of this contribution with the concentration of Tb ions is obvious in Fig. 1. In addition there is a contribution to the resistivity from electron-phonon scattering. We expect this contribution in all alloys to have a temperature dependence similar to that of YSb where there is no magnetic scattering, and to increase somewhat in magnitude on going from YSb to TbSb.

For the dilute systems ($c \ll 1$) the measured anomalous temperature dependence of the resistivity was previously[3,4] explained by a single-ion model in which the Tb ions scatter the conduction electrons independently, the total resistivity being simply the number of ions times the contribution from each ion. The electron-ion exchange interaction makes possible a variety of elastic and inelastic scattering processes. Due to the singlet nature of the ground state for a Tb ion in the cubic crystal field the contribution of these processes to the resistivity vanishes at zero temperature. At temperatures much greater than a characteristic energy splitting in the $4f$ multiplet it approaches a constant, the spin-disorder limit $\rho_{T \to \infty}$. At Tb concentrations above about 0.3 the ion-ion interaction begins to be important, and the single-ion model can no longer be used. When $c \gtrsim 0.4$ this interaction is strong enough to cause an antiferromagnetic transition. The observed Néel temperature is in good agreement with the one calculated in the molecular-field approximation applied to the full level scheme (we neglect in this work the sixth-order crystal field contribution). In the resistivity curves on Fig. 1, the transition is clearly identifiable in the alloys with $1 > c > 0.5$.

In the presence of an indirect exchange interaction between the ions the crystal field levels

broaden into bands of magnetic excitons. To calculate the resistivity in the spatially ordered alloy TbSb we treat the electron-ion interaction in the Born approximation and express the scattering cross section in terms of the imaginary part

of the ion-ion susceptibility function $\chi(\vec{q},\omega)$.[5] For the electron-ion exchange interaction we use the same spatially localized form as in Ref. 4. Since the Fermi surface of these alloys is unknown, we take it to be spherical. The resistivity may then be expressed as

$$\rho = \rho_0 \int_0^1 d\left(\frac{q}{2k_F}\right)\left(\frac{q}{2k_F}\right)^3 \int \frac{d\Omega_{\hat{q}}}{4\pi} \int_{-\infty}^\infty d(\hbar\omega)\, \frac{\hbar\omega/k_B T}{\sinh^2(\hbar\omega/2k_B T)}\, \frac{1}{\pi}\mathrm{Im}\chi(\vec{q},\omega). \tag{1}$$

ρ_0 is a constant proportional to the square of the electron-ion exchange constant. It is chosen such that $\rho_{T\to\infty} = J(J+1)\rho_0$, the spin disorder limit of the single-ion model.[4] The value of the Fermi momentum k_F is an important parameter in the calculation because it determines which excitons affect the resistivity. In particular if k_F is very small only the low-momentum excitons, whose energies are relatively higher than in the single-ion model, can scatter the electrons. Consequently the resistivity increases less rapidly towards its saturation value than predicted by the single-ion model. Confining ourselves to the paramagnetic regime we calculate $\chi(\vec{q},\omega)$ within the random-phase approximation with a pseudo-fermion representation of the crystal field states.[5] For simplicity we include only the lowest singlet (Γ_1), and the next two lowest triplets (Γ_4 and $\Gamma_5^{(2)}$) of the crystal field multiplet. This approximation to the level scheme is excellent in the temperature range considered ($T < 30$ K) since the next higher state in the multiplet (Γ_3) lies at 92 K. Our result for the susceptibility function corresponds to that obtained by Holden and Buyers[6] from an equation-of-motion method. In general the calculation of ρ from Eq. (1) must be performed numerically. In the absence of ion-ion interaction the resistivity becomes identical to that obtained in Ref. 4. In the actual calculation only next-nearest-neighbor interactions are taken into account and the ion-ion exchange parameter is chosen such that the result of the molecular field calculation of the transition temperature agrees with the experimentally observed value of 15.1 K.

For the alloys with $c < 1$, in which the Tb ions do not form a spatially periodic lattice, we shall assume that the excitonic modes are still reasonably well defined, and that their dispersion may be calculated approximately by letting the Tb ions be periodically distributed on a hypothetical lattice with a spacing proportional to $c^{-1/3}$. We then take the Tb concentration into account by multi

plying the ion-ion exchange parameter by c.[2] Furthermore we take $2k_F$ to be concentration independent and given by the value which yields the best overall fit, $2k_F = 0.6\pi/a$, where a is the lattice constant for the Tb lattice in TbSb. The result of the calculation is shown by the solid lines in Fig. 1. The curves have been fitted to experiment at 10 K, or just above T_N in cases where T_N exceeds 10 K. In fitting the curves for the alloys that order magnetically we have taken into account contributions to the residual resistivity from the disorder in the spatial configuration of the magnetic ions, as calculated within the molecular field approximation. At zero temperature this contribution vanishes as a function of concentration at $c = 1$ and at the critical concentration $c = 0.42$. In between it has a maximum equal to about 15% of $\rho_{T\to\infty}$ for the value of c in question.

We conclude that the experimental and theoretical results shown in Fig. 1 are in excellent agreement considering the crudeness of the model. The difference between the measured and calculated curves, similar in all alloys, is attributed to electron-phonon scattering. The only significant deviation of theory from experiment is seen at low temperature for the alloys of nearly critical concentration. This is hardly surprising since the magnetic properties of the system change very rapidly in this concentration regime. The agreement between our calculated electron-exciton resistivity and the experimental curves has been obtained by just one concentration independent choice of the Fermi momentum and a scaling of each theoretical curve in terms of absolute resistivity. However, there is the constraint that the high-temperature saturation value should scale with Tb concentration c (for the three-level scheme used here it turns out that this saturation value is only a few percent lower than the one calculated for the full multiplet). Thus from our fits we determine the high-tem
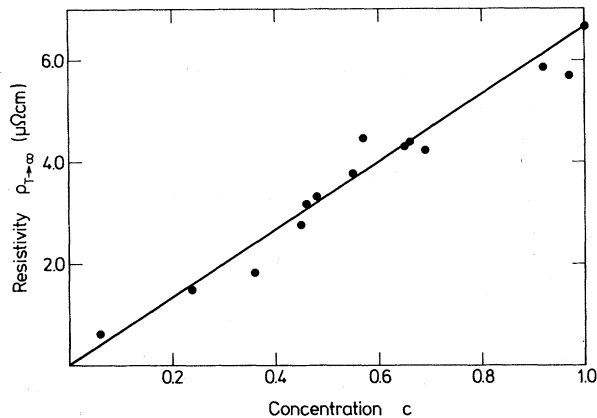
FIG. 2. The concentration dependence of $\rho_{T \to \infty}$ as determined from Fig. 1. The straight line indicates the theoretical prediction.

perature spin-disorder resistivity $\rho_{T \to \infty}$ for each concentration. In Fig. 2 we have plotted this $\rho_{T \to \infty}$ versus c. Indeed we find $\rho_{T \to \infty} \propto c$.

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X-Ray Photoemission from Lithium: An Explanation of Its X-Ray Edge

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Analysis of new Li 1s x-ray-photoemission data as a function of temperature unambiguously shows a *large* phonon-broadening contribution and a *small* lifetime width. Our values account *quantitatively* for the observed rounding in all the recent Li K absorption-edge measurements.

The rounded K-x-ray edge of lithium metal has been the source of controversy for almost thirty years. Following the theory of Mahan, Nozières, and De Dominicis (MND),[1,2] calculations[3-5] of the threshold exponent have all predicted a rounded edge, but one that was insufficiently broad[6] to explain the data.[7,8] This, along with the electron-scattering results by Ritsko, Schnatterly, and Gibbons,[9] has challenged the importance of the MND theory in explaining the Li measurements. Several years before that theory was questioned, McAlister,[10] using a model due to Overhauser,[11] suggested that a transition density of states

broadened by phonons could explain the data. Overhauser's model, however, also predicted phonon broadening of the Na edge in excess of the reported width in that material.[12] Bergerson, McMullen, and Carbotte[13] recalculated the phonon broadening for Li and Na and found them both to be considerably smaller than Overhauser's values, but both of comparable magnitude. Dow, Robinson, and Carver,[6] using a different mechanism, made estimates of large phonon broadening for Li and argued for a smaller broadening for Na. Their approach, rebutted by Bergerson, Jena, and McMullen[14] and by Mahan,[5] subsequent-