strong for (NMP)(TCNQ), where the experimental picture is most complete. The quinolinium salt is a metal at high temperatures; the low-temperature properties are not yet well understood. However, assuming the Q(TCNQ)$_2$ chains (with $\frac{1}{4}$-filled band) remain metallic, an upper limit on the chain length can be obtained from straightforward application of spin diffusion theory to determine the contribution to the proton T_1 from paramagnetic centers at the chain ends. The result is an estimated length of order 500 lattice constants. This estimate is in reasonable agreement with the interpretation of the Curie contribution to χ[13] as arising from paramagnetic defects at chain ends.

The sensitivity of 1D systems to disorder localization can be exploited by using TCNQ compounds. As a first example we show in Fig. 3 the inverse susceptibility of (NMP)$_{0.99}$(NEP)$_{0.01}$(TCNQ), where NEP denotes *N*-ethyl-phenazinium. The substitution of C$_2$H$_5$ for CH$_3$ on 1% of the cations has clearly observable effects. The "transition" appears to be somewhat rounded and shifted, but the major change is in magnitude. The high-temperature Pauli term is decreased in the disordered mixed crystal consistent with a spread of localized-state energies somewhat greater than the pure-system intrinsic bandwidth. The low-temperature magnetism is also decreased relative to that of the pure system as expected with increased disorder.[12,14] The disorder in this mixed (NEP)-(NMP) system probably arises from the steric effect of the larger ethyl group. The observation of a clear effect with only 1% NEP indicates that in the pure (NMP)(TCNQ) the wave functions extend to distances far greater than the length of order a lattice constant predicted by BWV. More detailed studies of the effect of *controlled* disorder are in progress and will be published separately.

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Contribution of Nonparabolicity to Longitudinal Magnetoresistance at Quantum Magnetic Fields

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In this communication we report that in the quantum region of magnetic field ($\hbar\omega_c \gg k_BT$) the nonparabolicity alone leads to a nonzero longitudinal magnetoresistance even if the energy and magnetic-field dependence of the relaxation time is ignored.

It is well known that anisotropy in the band structure of semiconductors gives rise to longitudinal effects, viz., longitudinal magnetoresistance. In the quantum region of magnetic field, i.e., where $\hbar\omega_c \gtrsim k_BT$, the dependence of electron collision frequency on electron energy and applied magnetic field also gives rise to longitudinal magnetoresistance[1] even in a semiconductor which has parabolic and isotropic energy bands. In this communication we predict a nonzero longitudinal magnetoresistance (LMR) in the quantum region of magnetic field, which arises solely because of the nonparabolicity of the energy bands. For the sake of simplicity we shall assume that the magnetic field is strong enough to confine most of the electrons in the lower energy state, i.e., $n=0$; this is always true for magnetic fields for which $\hbar\omega_c \gg k_BT$. The theory presented here is applicable to group III-V compounds which are known to have marked nonparabolicity. The analysis assumes that the semiconductor has nonparabolic energy bands in which the constant-energy surfaces in k space are spheres. The relaxation time for electron collisions is assumed to be independent of electron energy as well as of magnetic field. Using Kane's model[2] for small-gap semiconductors and taking into account the quantization of energy levels introduced by a strong longitudinal magnetic field, we derive the expression for LMR. We have calculated LMR for various values of magnetic field and band gap and the results have been presented in the form of graphs. It is seen from our calculations that LMR decreases with increasing band gap but increases with increasing magnetic field.

The energy of an electron in a nonparabolic band in the presence of a quantizing longitudinal magnetic field can be expressed as[3]

$$\epsilon \cong -\tfrac{1}{2}\epsilon_g + \tfrac{1}{2}\epsilon_g a_n + \tfrac{1}{2}\hbar^2 k_z^2/m_n a_n, \tag{1}$$

where

$$a_n = (1 + 2\hbar\omega_c/\epsilon_g)^{1/2}. \tag{1a}$$

ϵ_g is the band gap, m_n is the effective mass at the band edge, ω_c is the cyclotron frequency, and k_z is the electron wave vector along the direction of the magnetic field. From Eq. (1) it is easy to see that effective mass m^* is given by

$$m^* = m_n a_n. \tag{2}$$

Following Argyres and Adams and using Eq. (2) for the effective mass of electron, we get the following expression for $\rho(H)$, the electrical resistivity in the presence of a very strong longitudinal magnetic field

$$\rho(H) = m_n a_n / ne^2\tau_0. \tag{3a}$$

The electrical resistivity in the absence of a magnetic field is given by[4]

$$\rho(0) = \frac{3m_n}{2ne^2\tau_0} \frac{\int_0^\infty y^{1/2} y' e^{-x}\,dx}{\int_0^\infty y^{3/2}(y')^{-1} e^{-x}\,dx} = \frac{3m_n}{2ne^2\tau_0}\frac{I_1}{I_2}, \tag{3b}$$

with

$$y = (\epsilon/k_BT)(\epsilon/\epsilon_g + 1),$$
$$y' = 1 + 2\epsilon/\epsilon_g; \tag{4a}$$

x is the normalized energy, $-e$ is the electronic charge, n is the electron density of sample, and τ_0^{-1} is the electron collision frequency which has been assumed to be independent of electron energy and magnetic field.

From (3a) and (3b) one obtains the following expression for the fractional change in resistivity:

$$\frac{\Delta\rho}{\rho_0} = \frac{\rho(H) - \rho(0)}{\rho_0} = \frac{2}{3} a_n \frac{I_2}{I_1} - 1. \tag{5}$$

One can see from Eq. (5) that for a parabolic case, i.e., ($\epsilon_g \to \infty$, $y' \to 1$, and $y \to \epsilon/k_BT$) the longitudinal magnetoresistance, i.e., $\Delta\rho/\rho_0$ vanishes.

The variation of LMR, i.e., $\Delta\rho/\rho$, with dimensionless magnetic field $\hbar\omega_c/k_BT$ is shown in Fig. 1 for various values of normalized band gap ϵ_g/k_BT. It is noted from Fig. 1 that LMR increases with increasing magnetic field but decreasing band gap (i.e., increasing nonparabolicity). This can be explained as follows. In a nonparabolic semiconductor the effective electron mass is a function of electron energy. By the application of a high magnetic field ($\hbar\omega_c/k_BT \gg 1$) the electron energy becomes quantized and therefore the effective mass of the electron becomes a function of magnetic field also. This dependence of electronic mass on magnetic field [as given by Eq. (2)] gives rise to a nonzero LMR which increases

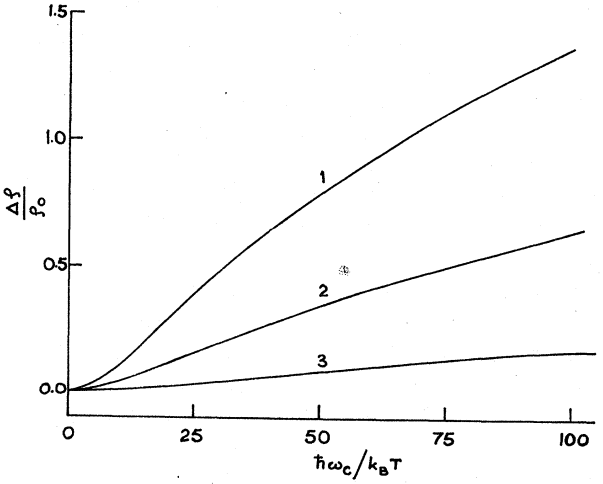

FIG. 1. Variation of fractional change in resistivity, $\Delta\rho/\rho_0$, with magnetic field $\hbar\omega_c/k_BT$ for various values of ϵ_g/k_BT. Curves 1, 2, and 3 are for $\epsilon_g/k_BT = 30$, 100, and 500, respectively.

with decreasing ϵ_g/k_BT and increasing $\hbar\omega_c/k_BT$.

It may be pointed out here that the present analysis is valid only for the case of very strong magnetic fields. This is because of the fact that Eq. (1) is true only for $\hbar\omega_c \gg k_BT$. Furthermore, our theory accounts only for LMR due to the nonparabolicity of the energy bands. No account has been made for the LMR due to magnetic-field-dependent relaxation time; but this was done only to emphasize the contribution of nonparabolicity to LMR. A theory which accounts for both of these sources which contribute to LMR is being worked on and the results shall be reported in a future communication.

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Evolution of Core States from Energy Bands in the 4*d*5*s*5*p* Region from Pd to Xe †

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X-ray photoemission studies were performed on the $4d5s5p$ elements Pd through Te using monochromatized Al ($K\alpha$) radiation. With increasing atomic number the $4d$ structure evolves from d bands to spin-orbit—split atomiclike core levels. Structure was observed in the $5s5p$ bands for the first time by this method. The cohesive energy was attributed to the $5p$ bands in In through Sb. Evidence for both bonding and nonbonding $5p$ bands was obtained for Te.

Most discussions of band structure in metals are predicated on the assumption that the tightly bound electrons can be regarded as belonging to separate ion cores, while those that are more loosely bound occupy valence bands. In passing beyond the end of a transition series one would expect the d bands to become narrower, fall below the Fermi energy E_F, and evolve into core levels. It is not always clear, however, just which atomic levels can be safely treated as core states and which ones must be explicitly included as part of the band structure. In this Letter we report x-ray photoelectron spectroscopy (XPS)[1] experiments addressed to this question for the $4d5s5p$ elements Pd ($Z = 46$) through I ($Z = 53$). By following the $4d_{3/2}$-$4d_{5/2}$ spin-orbit splitting from I down through Cd to Ag, one can unambiguously trace the onset of band-structure broadening. We also report the first observation by XPS of structure in the sp bands. This structure exhibits systematic changes between Cd and Te.

The specimens studied were high-purity single crystals in each case except Sb and I, for which polycrystalline samples were used. All the specimens except I were studied in a Hewlett Packard 5950A spectrometer with a monochromatic Al ($K\alpha$) x-ray source. The working pressure was always less than 5×10^{-9} Torr. Iodine was examined in the Berkeley iron-free spectrometer. Standard metallographic methods were used to produce clean surfaces. The typical procedure consisted of spark-cutting disks from single-crystal rods, mechanically polishing, and finally electropolishing just prior to insertion into the vacuum chamber. Surface purity was monitored *in situ*, and the sample was repeatedly argon etched until all impurity XPS lines were eliminated. This typically required 15 min of bombardment with a 10-μÅ beam of 900-V Ar$^+$ ions. Oxygen 1s and carbon 1s spectra taken after each valence-band measurement indicate that there was no oxygen buildup. A carbon layer corresponding to $\frac{1}{10}$ the intensity of the carbon 1s line of graphite accumulated on the surface after 10 h.

Valence-band spectra are displayed in Fig. 1, and derived parameters are set out in Table I.