edge. This narrow resonance indicates that a discrete ($3d^8 4s$) final state exists for Cu with the $4s$ electron localized at the site of the $3d$ holes. This calls into question models treating the shakeup electron (nl in Fig. 3) as itinerant.[3] The magnitude of the satellite cross sections is ~ 7 times larger in Ni than in Cu. This indicates the contribution of extra shakeup levels due to empty d states ($nl = 3d$), for Ni compared with Cu.

We expect that the two-electron resonance observed for Cu and Ni occurs for d levels in other materials, especially for higher-Z atoms where atomic effects become important.[7] Compared with Ni, Cu is a simpler test case for studying many-electron effects at the $3p$ threshold because of its sharp atomiclike[7,10] satellite and Auger multiplets and the simple filled-d-shell ground state.

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Anomalous Magnetoresistance of Quasi One-Dimensional $Hg_{3-\delta}AsF_6$

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Resistivity and magnetoresistance data in the field range 0–180 kG at low temperatures are presented. The temperature dependence (T^3), suppression of residual resistance, and large magnetoresistance are understood as resulting from the unusual Fermi surface. In spite of the large number of defects and the relatively weak interchain coupling ($\Delta\epsilon/E_F \sim 10^{-2}$) inferred from the magnetoresistance, the states near E_F are extended over distances greater than 100 μm.

The incommensurate linear chain structure of $Hg_{3-\delta}AsF_6$ leads to unique one-dimensional (1d) lattice dynamics[1] and highly anisotropic electronic properties.[2-4] Transport studies showed metallic behavior with $\rho_{ab}(300\text{ K}) \simeq 10^{-4}$ Ω-cm and no sign of residual resistivity,[3] a result of particular interest since the unusual structure[1,5] contains approximately 6% anion vacancies.[6] The magnetoresistance[4] is large in low fields, and the increment, $\Delta\rho(T,H) \simeq \Delta\rho(H)$, is insensitive to temperature. These magnetoresistance data were described in terms of a magnetic-field-induced residual resistivity.[4]

We present new data on the resistivity and magnetoresistance in the extended field range 0–180 kG at low temperatures. Low-field studies show that $\Delta\rho/\rho(0)$ approaches quadratic behavior only for $H \lesssim 1$ G. The high-field results show no saturation for $\rho(H)$ and demonstrate that although $\rho(T,0)$ varies strongly with temperature ($\sim T^3$ for $T<30$ K), $\Delta\rho(H)$ is insensitive to T. We propose a theoretical explanation of the resistivity and magnetoresistance based on the unusual Fermi surface which results from the perpendicular sets of linear Hg chains.

All magnetoresistance data were obtained by an improvement on the contactless ac technique described in Ref. 4. The low-field data for $\rho_{ab}(H)$ at 4.2 K are shown in Fig. 1. Since the line on the log-log plot has slope 2, $\Delta\rho/\rho(0)$ approaches an H^2 dependence only at the lowest fields. The inset plots the same data as $[\Delta\rho/\rho(0)H^2]^{1/2}$ versus H. An effective magnetoresistance mobility can be obtained from the low-field limit:

$$\mu_{\mathrm{eff}} \equiv \lim_{H\to 0}\left(\frac{\Delta\rho}{\rho_0 H^2}\right)^{1/2} \simeq 5\times 10^5\ \mathrm{cm^2/V\,s}. \qquad (1)$$

The transport mobility (μ) is obtained directly from the conductivity, $\sigma = ne\mu$, where n is the number of carriers with charge $|e|$. With use of cross sections of the Fermi surfaces[7] of the two zeroth order bands (ϵ and γ), one calculates $n = \sum n_i \simeq 3.9\times 10^{21}$ cm^{-3}. The measured value, $\sigma(4.2\ \mathrm{K}) = 2.8\times 10^7$ $(\Omega\ \mathrm{cm})^{-1}$, then yields $\mu = 4.5 \times 10^4$ cm^2/V s. Note that the magnetoresistance μ_{eff} is enhanced over μ by an order of magnitude. The mean free path implied by $\mu = 4.5\times 10^4$ cm^2/V s is $\lambda \simeq 50$ μm assuming a free-electron mass.[2,7] Since $\rho_{ab}(T)$ does not become residual even at 1.2 K, the impurity or defect scattering λ can be conservatively estimated as >100 μm.

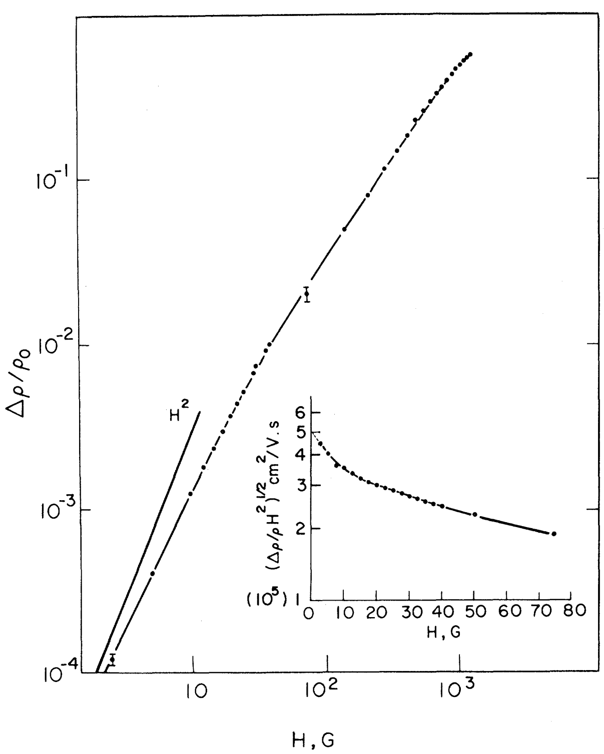

FIG. 1. $\Delta\rho/\rho_0$ vs H at 4.2 K on a log-log scale. The line is H^2 dependence. Inset: $\mu_{\mathrm{eff}} \equiv (\Delta\rho/\rho_0 H^2)^{1/2}$ vs H.

Figure 2 shows the $\hat{a}$-$\hat{b}$ plane magnetoresistance at low temperatures. Although the quadratic region (Fig. 1) is limited to $H<1$ G, $\rho(H)$ does not saturate even at 180 kG (Fig. 2). At high fields $\rho(H)$ is essentially temperature independent consistent with the field-induced residual resistivity.[4] The temperature dependence of ρ_{ab} ($H=0$, $T<30$ K) is shown in the inset. These high-precision dc resistivity data were obtained with use of the Montgomery technique[3] on a carefully prepared flat planar crystal. The solid line represents T^3 behavior.[4]

An understanding of the Fermi surface (FS) of $Hg_{3-\delta}AsF_6$ is crucial to the magnetoresistance. Ehrenfreund *et al.*[8] found a cylindrical surface with nearly square cross section, but with rounded corners arising from weak interchain coupling. Razavi *et al.*[7] reported de Haas–Van Alphen results from which they inferred a FS consisting of a series of cylinders with axes along $\hat{c}^*$ (Fig. 3). They conjectured that these cylinders were the result of filling up 1d states in k space; the

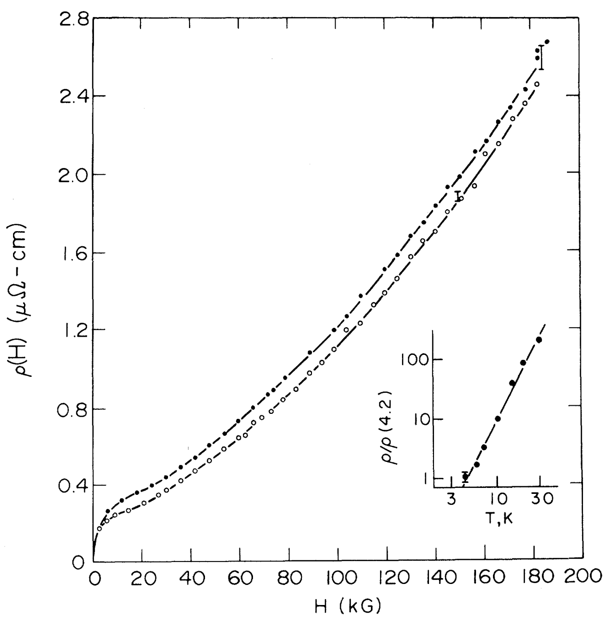

FIG. 2. $\rho(H)$ vs H at 4.2 K (upper curve) and 1.8 K (lower curve). Inset: $\rho(T,0)/\rho(4.2,0)$ vs T on a log-log scale. The line represents T^3 dependence.

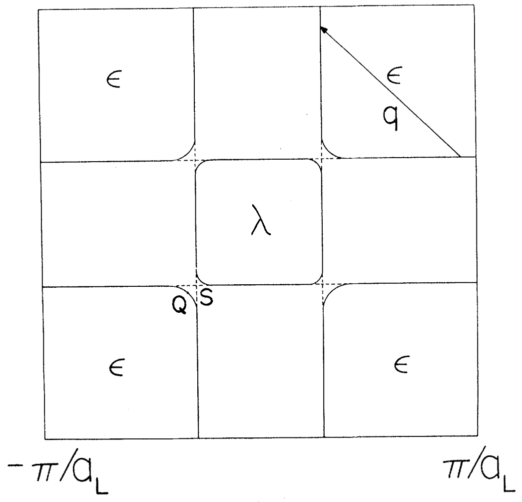

FIG. 3. Fermi surface of $Hg_{3-\delta}AsF_6$ after Razavi *et al.* (Ref. 7). The dashed line is in the limit of no interchain coupling.

dashed line is the FS in the absence of interchain coupling. Weak interchain coupling removes the degeneracy at the corners as described by Ehrenfreund *et al.*[8] The interchain coupling ($\Delta\epsilon$) leads to rounded corners over a region Δp such that $\Delta\epsilon/E_F = \Delta p/p_F$. The small parameter, $x = \Delta p/p_F$, is the fraction of the FS that is curved; the remainder of the FS is nearly flat. Only in the corners does the wave function have significant amplitude on both sets of chains. On the flat regions, it is localized in real space on any one family of chains.

The topological features of this Fermi surface place severe restrictions on impurity and phonon scattering. We assume, as a model, that impurities and defects are ineffective on the planar sections giving a long scattering time τ_p, but they are fully effective on the corners giving a short scattering time τ_c; $\tau_p \gg \tau_c$. This assumption[9] is in agreement with the apparent absence of residual resistivity in the presence of ~6% anion vacancies. In zero field, $\rho = (m/ne^2)[x\tau_c + (1-x)\times\tau_p]^{-1} \simeq m/ne^2\tau_p$, where m is approximately the free electron mass.[2,7] If $\tau_p \gg \tau_c$, the residual resistance is suppressed in agreement with the zero-field resistivity data. A similar argument was recently presented by Kaveh and Ehrenfreund[10] to predict a T^3 dependence for $\rho_{ab}(T)$ from phonon scattering at low temperatures, in good agreement with the observed dependence (Fig. 1).

This two-relaxation-time model leads to a phenomenological explanation of the unusual magnetoresistance. For $H = 0$, the planar and corner regions act "in parallel," and σ is determined by τ_p; the corners are essentially shorted out. When $H \neq 0$, the carriers traverse p-space orbits on the FS perpendicular to the field. For $\vec{H} \parallel \vec{c}$, the Lorentz force transfers carriers into the corners where they are rapidly scattered. In effect, the magnetic field puts the corner and planar regions "in series" and in high fields subjects *all* the carriers to the fast corner scattering rate. If impurity and defect scattering dominate τ_c^{-1}, $\Delta\rho(H, T)$ will be independent of T in agreement with the field-induced residual resistivity.[4] For H in the $\hat{a}$-$\hat{b}$ plane, however, no such transfer of carriers into the corners occurs, and one expects a weak magnetoresistance. In this configuration (both H and the current in the a-b plane), we find that any magnetoresistance is <1% at 4.2 K and 1 kG. Thus, as a result of the unusual FS, the magnetoresistance can be understood as a Lorentz-force effect, contrary to our earlier belief.[4]

We have analyzed the path-integral formula[11] for $\rho(H)$ with a cylindrical FS in the two-relaxation-time approximation outlined above, with use of the model band structure of Ehrenfreund *et al.*[8] It is convenient to separate four regions: (1) very low fields $\tau_p/x \ll T$, (2) intermediate low fields $\tau_p \ll T \ll \tau_p/x$, (3) intermediate high fields $\tau_c/x \ll T \ll \tau_p$, and (4) very high fields $T \ll \tau_c/x$.

In the weak-field limit we obtain

$$\frac{\Delta\rho(H)}{\rho(0)} \sim x\left(\frac{\tau_p}{xT}\right)^2 \sim \frac{1}{x}(\mu H)^2, \tag{2}$$

where μ is the conductivity mobility. An analogous result was obtained[12] earlier for a FS model consisting of a cube with rounded edges and corners. Equation (2) implies $x \simeq (\mu/\mu_{\mathrm{eff}})^2 \simeq 10^{-2}$ [see Eq. (1)]. Since $x \sim \Delta\epsilon/E_F$ the interchain coupling is estimated as $\Delta\epsilon \sim xE_F \simeq 0.04$ eV. This weak interchain coupling is a measure of the quasi one-dimensionality of $Hg_{3-\delta}AsF_6$.

In the high-field limit, $T \ll \tau_c/x$, and the carriers complete many orbits between collisions. Restricting ourselves to fields below magnetic breakdown where there are no open oribts, we expect $\rho(H)$ to saturate at the value $mx/ne^2\tau_c$ due to scattering of all the carriers at the corner where the probability of scattering is of order x/τ_c. The data suggest an approach to saturation near 20 kG (see Fig. 2 and Ref. 5) with a subsequent increase in $\rho(H)$ at higher fields. This high-field increase in $\rho(H)$ and the absence of saturation at fields as high as 180 kG may result from magnetic breakdown. In any case $\Delta\rho/$

$\rho(0) > 10^2$ at (1.8 K, 20 kG) so that we conservatively estimate $\tau_c < 10^{-2} x \tau_p$. The suppression of residual resistivity in the planar regions is quite strong.

In regime (3), $\tau_c/x \ll T \ll \tau_p$, and the carriers are scattered only on the corners, which can be regarded as scattering points. The conductivity tensor is diagonal (to order H^{-1}) so that $\rho(H) \simeq |H/nec|$. In this intermediate field regime, the Hall effect is predicted to be zero; the carriers are rapidly scattered at the corners so that there is no transverse current and hence no Hall effect.[12] Using the linear part of the data in Fig. 1 we estimate $n \simeq 6\times10^{21}/\mathrm{cm}^3$, compared with $3.9\times10^{21}/\mathrm{cm}^3$ which is the sum of the carrier densities in the ϵ and γ bands.[7] The agreement is satisfactory, considering the simplicity of the model.

In (2) the fraction (τ_p/T) of carriers affected by the field is small, but nevertheless large compared with x. The corners still appear sharp, and one obtains $\Delta\rho/\rho_{(0)} \sim \tau_p/T$ so that $\Delta\rho \sim H/nec$. Here, too, the Hall effect is predicted to be zero. Note that $\Delta\rho$ is temperature independent except in the lowest field (H^2) regime.

This discussion provides a starting point towards understanding the remarkable transport properties of the quasi-1d Hg-chain system. The extension to more than one band is conceptually routine, $\sigma = \sum_n \sigma_n$, where n is the band index. However, this introduces more parameters since τ_p and x are expected to be correlated to the detailed shape of the FS. Even if all τ's are known, one must contend with the complexity of the FS introduced by the incommensurability between the Hg and AsF_6^- sublattices.[1,6,7]

In conclusion, analysis of the unusual magnetoresistance of $Hg_{3-\delta}AsF_6$ has resulted in evaluation of the strength of interchain coupling; $\Delta\epsilon/E_F \sim 10^{-2}$, implying that the electronic structure is quasi-one-dimensional. The experimental results imply that the flat planar Fermi surface inhibits impurity and defect scattering and thereby leads to a magnetic-field-dependent residual resistance. The large mean free path (>100 μm) inferred from the magnitude of the conductivity sets a lower limit on any localization length in this quasi-1d metal.

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