Observable resonant states of iron in $Fe_xHg_{1-x}Se$ crystals

P. N. Gorleĭ, V. N. Makogonenko, S. Yu. Paranchich, and L. D. Paranchich
Chernovtsy State University

(Submitted 16 September 1989)
Pis'ma Zh. Eksp. Teor. Fiz. **50**, No. 8, 348–350 (25 October 1989)

Measurements of the temperature dependence of the thermal emf in $Fe_xHg_{1-x}Se$ single crystals in a classically strong magnetic field have revealed a structural feature in the state density of the conduction band. This feature is interpreted as a narrow band of allowed states which are a consequence of the presence of iron.

1. In an effort to carry out a detailed investigation of the properties of narrow-gap semimagnetic solid solutions based on the telluride and selenide of mercury with *d* or *f* elements, we have carried out a thorough study of the temperature dependence of the thermal emf of several $Fe_xHg_{1-x}Se$ samples over the temperature range 77–400 K.

 0021-3640/89/200377-04$01.00

The measurements were carried out in magnetic fields up to 1.2 T. The test samples were cut from bars of unoriented single-crystal samples grown by the Bridgman method with electron densities $n = 9.4\times10^{23} - 5.6\times10^{24}\ \mathrm{m}^{-3}$ in the composition interval $0.01 \leqslant x \leqslant 0.2$.

2. Analysis of the results of the measurements shows that all the samples exhibit an anomalous feature which is not characteristic of pure mercury selenide on the temperature dependence of the thermal emf in an infinite (nonquantizing) magnetic field in the temperature range 77–400 K. This anomalous feature can be attributed to the presence of a resonant level in the band of allowed energies of the $Fe_xHg_{1-x}Se$ band structure.

3. Figure 1 illustrates the experimental results with results on the temperature dependence of the electrical conductivity σ (curve 1), the Hall coefficient R (curve 2), the thermal emf in the absence of a magnetic field (α_0; curve 3); and the thermal emf in a classically strong magnetic field (α_∞; curve 4) for samples of $Fe_{0.01}Hg_{0.99}Se$. The values of α_∞ were determined from the Rodot relation[1] within a relative error $\sim5\%$. We see that $\sigma(T)$ and $R(T)$ fall off smoothly, and $\alpha_0(T)$ increases smoothly, with increasing temperature. On the curve of $\alpha_\infty(T)$, on the other hand, there is an abrupt change in slope at $T\approx210$ K.

4. In the case of a highly degenerate carrier gas, as in the present experiments, the quantity α_∞ can be expressed in terms of the electron density n, the temperature T, and the electron state density (per unit volume) at the Fermi level, $\rho(\varepsilon_F)$, as follows[2]:

$$\alpha_\infty = \frac{2}{3}\,\frac{\pi^2 k_B^2\, T\rho(\epsilon)}{en}\,. \qquad (1)$$

From expression (1) and the experimental data on the temperature dependence

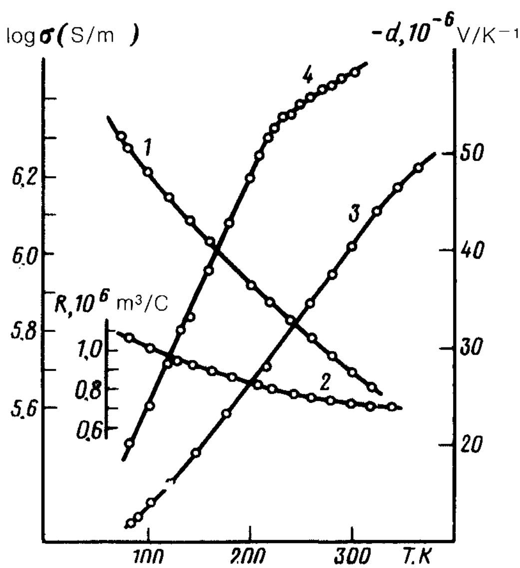

FIG. 1. Temperature dependence of (1) the electrical conductivity σ, (2) the Hall coefficient R, (3) the thermal emf α_0, and (4) the magnetothermal emf α_∞ of samples of $Fe_{0.01}Hg_{0.99}Se$ solid solutions.

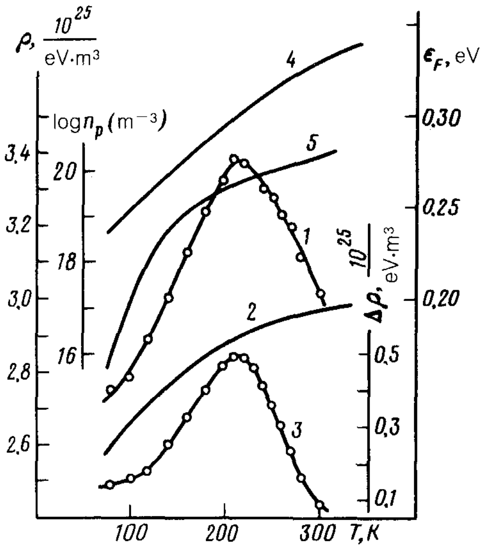

FIG. 2. Temperature dependence of the state density in $Fe_{0.01}Hg_{0.99}Se$ solid solutions. 1—$\rho_{expt}(\varepsilon_F)$; 2—$\rho_{band}(\varepsilon_F)$; 3—$\Delta\rho(\varepsilon_F)$; 4—the Fermi energy ε_F; 5—the carrier density in the resonant level, n_p.

$\alpha_\infty(T)$ and $n(T)$ we can determine the experimental temperature dependence of the state density, $\rho_{expt}(\varepsilon_F)$; the result is shown by curve 1 in Fig. 2. If we assume that the band parameters of the $Fe_xHg_{1-x}Se$ solid solution differ only negligibly from those of pure mercury selenide for the composition $x = 0.01$, and if we use data from the literature[3] on HgSe in the approximation of the Kane two-band model, we can calculate the Fermi energy (curve 4 in Fig. 2) and the density of band electron states, $\rho_{band}(\varepsilon_F)$ (curve 2 in Fig. 2). The difference $\Delta\rho(\varepsilon_F) = \rho_{expt}(\varepsilon_F) - \rho_{band}(\varepsilon_F)$, shown by curve 3 in Fig. 2, is naturally linked with the state density of the resonant level of iron in the energy band of a band electron.

5. The bell-shaped curve of $\Delta\rho(\varepsilon_F) = f(T)$ implies the following model expression for this dependence[4]:

$$\Delta\rho(\epsilon_F) = \frac{N_p}{\pi}\frac{\Gamma}{[(\epsilon_F - E_p)^2 + \Gamma^2]}, \tag{2}$$

where N_p is the density of impurity centers in the resonant level, and E_p and Γ are the depth and half-width of the resonant level itself. Using data on $\Delta\rho(\varepsilon_F)$, we can estimate the values of the parameters in (2); we find

$$E_p = (0.294 \pm 0.05)\,\mathrm{eV}; \quad N = 3.96\cdot 10^{23}\,\mathrm{m}^{-3}; \quad \Gamma = (0.023 \pm 0.02)\,\mathrm{eV}. \tag{3}$$

These results agree fairly well with the data in the literature on E_p (Ref. 5), and they yield an estimate of the lifetime of an electron in a state with an energy E_p:

$$\tau_p \approx \hbar/\Gamma = 3\cdot 10^{-14}\,\mathrm{s}.$$

6. A question which naturally arises is just why the resonant level is not reflected on the temperature dependence of the electrical conductivity or that of the Hall coeffi-

cient (Fig. 1). We used (3) to calculate the carrier density in the resonant level, from the formula

$$n_p = \int_0^\infty \Delta\rho(\epsilon_F) f_0(\epsilon) d\epsilon, \tag{4}$$

where $f_0(\varepsilon) = [1 + \exp(\varepsilon - \varepsilon_F + E_p/kT)]^{-1}$ is the Fermi–Dirac function. The energy is reckoned from the bottom of the conduction band. It turns out that over the entire temperature range studied the quantity n_p (curve 5 in Fig. 2) is lower than the density of band electrons by more than four orders of magnitude.

The significant difference between the densities of band carriers and "resonant" carriers, combined with the fact that σ and R are comparable in magnitude in our case, suggests that coherent scattering makes an unimportant contribution to the values of σ and R for $Fe_{0.01}Hg_{0.99}Se$ crystals. More-definitive conclusions will have to await a specific numerical calculation.

[1]M. Rodot, Ann. Phys. (Paris) **5**, 1083 (1960).

[2]I. M. Tsidil'kovskiĭ, *Band Structure of Semiconductors*, Nauka, Moscow, 1978, p. 327.

[3]K. Leibler *et al.*, Phys. Status Solidi B **47**, 405 (1971).

[4]I. M. Tsidil'kovskiĭ *et al.*, *Impurity States and Transport Phenomena in Gapless Semiconductors*, UNTs Akad. Nauk SSSR, Sverdlovsk, 1987, p. 141.

[5]N. G. Gluzman *et al.*, Fiz. Tekh. Poluprovodn. **20**, 1994 (1986) [Sov. Phys. Semicond. **320**, 1251 (1986)].

Translated by Dave Parsons