Fluctuation model of a gap-free semiconductor

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A model of a gap-free semiconductor without electrically active impurities (donors or acceptors) is proposed. Free electrons and weakly localized holes result from the Gaussian random potential. The Fermi level in this model depends weakly (logarithmically) on the pressure. The relationship between the electron mobility and the electron density is found.

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Gap-free semiconductors frequently contain residual electrons at low temperatures and exhibit a metallic conductivity. In a strong magnetic field, holes are sometimes also detected. One such semiconductor is a solid solution $Cd_xHg_{1-x}Te$ with $x<0.16$. The presence of residual electrons was originally attributed to a band overlap, which is allowed by the symmetry of the crystal.[1] The primary objection to this explanation is that the residual density varies markedly from sample to sample. The behavior of the samples with the high residual electron density can be attributed to the presence of a donor impurity. At low densities (10^{14}–10^{15} cm^{-3}), however, this explanation does not work, since these are the samples in which holes are found. Furthermore, a hydrostatic compression, which reduces the effective electron mass, causes the electron density in the samples to change in such a manner that the Fermi energy remains approximately constant. In the donor model, the density does not change.

Several investigators[2–4] have pursued the model of a highly compensated and highly doped semiconductor which was first proposed by Elliot *et al.*[2] Those studies suffer from the assumption of an exceedingly narrow impurity band, which does not correspond to certain calculations.[5]

In the present letter we consider a model without any electrically active impurities at all. Free electrons and weakly localized holes result from a random potential of the Gaussian type. A potential of ths type unavoidably arises in substitutional solid solutions because of fluctuations in the composition. In other situations a potential of this type might result from electrically inactive impurities or defects. For simplicity, we assume the potential $V(r)$ to be a white noise,

$$< V(r)\, V(r') > \; = \gamma\delta(r-r'). \tag{1}$$

the parameter γ is the sole characteristic of the fluctuation potential, so we can express the electron density, the electron mobility, and all the other kinetic coefficients in terms of this parameter. By eliminating γ we can thus find an expression which directly relates the mobility to the density.

Since the electron mass m_e is much smaller than the hole mass m_h, the fluctuation potential creates hole levels in the conduction band with a relatively small width

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Γ, while no electron levels appear in the valence band at all.[6] We define $g_h(E)$ to be the density of fluctuation states in the conduction band in the approximation $m_e = 0$. This density differs only by numerical coefficients from that corresponding to a simple band, and at high energies it can be written

$$g_h(E) = \frac{C}{E_0}(m_h E/\hbar^2)^{3/2}\exp(-\sqrt{E/E_0}), \quad (2)$$

where C is a numerical coefficient, $E_0 = 1.5\times 10^{-4}\gamma^2 m_h^3/\hbar^6$ according to the calculations of Ref. 7. Expression (2) was derived by an optimal fluctuation method[5] and is valid at $E \gg E_0$. Furthermore, the energy must be greater than or on the other of the binding energy of an acceptor, so that the exchange interaction can be ignored.[8,9]

Let us find the position of the Fermi level at $T = 0$. If it were at the top of the valence band [as it is in the case $V(r) \equiv 0$], the number of fluctuation holes would exceed the number of electrons. Accordingly, the condition of electrical neutrality lifts the Fermi level up into the conduction band. Electrons appear in the sample, and their charge cancels the charge of the holes in the fluctuation levels. As will be seen below, the Fermi level lies in an energy interval where the density of electron states can be considered unperturbed. The Fermi energy can be determined by equating the electron density (for simplicity, we use the parabolic approximation) to the density of the local hole states which arise in the conduction band,

$$\frac{1}{3\pi^2\hbar^3}(2m_e E_F)^{3/2} = \int_{E_F}^{\infty} g_h(E)\,dE. \quad (3)$$

We thus find, with logarithmic accuracy,

$$E_F = E_0 \ln^2[C_1(m_h/m_e)^{3/2}], \quad C_1 \simeq \frac{3\pi^2 \cdot 65}{\sqrt{2}} C, \quad (4)$$

and the residual density is

$$n = \frac{1}{3\pi^2\hbar^3}(2m_e E_0)^{3/2}\ln^3[C_1(m_h/m_e)^{3/2}]. \quad (5)$$

Since $E_F > E_0$, the electrons form a dense, degenerate gas and are distributed uniformly over the sample. The heavy holes, on the other hand, are localized at fluctuations, whose density is low. It can be seen from (4) and (5) that a change in m_e (caused by the pressure, for example) will cause the electron density to change far more than the Fermi level.

To calculate the mobility we note that since the localized states lie in the conduction band they have a width Γ, which is given in the case $F = E_F$ by[6] $\Gamma = C_2 E_F (m_h/m_e)^{3/2}$, where C_2 is a numerical coefficient. At $T = 0$ the most important electron-scattering mechanism is resonant scattering by localized states. The density (N) of localized states at resonance with electrons at the Fermi level is $g_h(E_F)\Gamma$, and the cross section for the resonant scattering is $\sigma = 2\pi\hbar^2/(m_e E_F)$ (which is a factor of m_h/m_e larger than the square of the radius of the localized state). The mean free path is $l = 1(N\sigma)$. We thus find the following expression for the mobility:

$$\mu = (2^{3/2}\,\pi C_2)^{-1}\, e m_h^{3/2} \,/(\hbar^2 m_e\, g_h(E_F)\sqrt{E_F}). \tag{6}$$

Combining (5) and (6), we can relate the electron mobility to the electron density:

$$\mu = \frac{(3\pi^2)^{1/3}}{2\pi C_2}\, \ln^{-1}[C_1(m_h/m_e)^{3/2}]\frac{e^2}{\hbar n^{2/3}}\left(\frac{m_h}{m_e}\right)^{3/2}. \tag{7}$$

Since expression (7) contains some unknown numerical coefficients, we can find only an order-of-magnitude estimate of the mobility. For HgTe we find $\mu \sim 10^5$–10^6 cm^2/(V s) at $n = 10^{15}$ cm^{-3}; this result corresponds to the data in Ref. 10. It was shown in Ref. 10 that the mobility falls off very rapidly with increasing density, apparently implying a scattering by charged impurities. This effect cannot be described by our model. We note that our assumption in (1) that the fluctuations constitute a white noise has no qualitative effect on the picture drawn above, simply affecting the logarithmic factors in Eqs. (4), (5), and (7).

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[1]P. I. Baranskiĭ, V. P. Klochkov, and I. V. Potykevich, Poluprovodnikovaya élektronika. Spravochnik (Handbook of Semi-Conductor Electrons), Naukova Dumka, Kiev, 1975.

[2]C. T. Elliot, J. Melngailis, T. C. Harman, J. A. Kafalas, and W. C. Kernan, Phys. Rev. **B5**, 2985 (1972).

[3]N. B. Brandt, O. N. Belousova, L. A. Bovina, V. I. Stafeev, and Ya. G. Ponomarev, Zh. Eksp. Teor. Fiz. **66**, 330 (1974) [Sov. Phys. JETP **39**, 157 (1974)]; L. A. Bovina, N. B. Brandt, S. V. Dolbanov, V. V. Evseev, V. I. Stafeev, and Ya. G. Ponomarev, Zh. Eksp. Teor. Fiz. **84**, 1453 (1983) [Sov. Phys. JETP [to be published)].

[4]Yu. G. Arapov, B. B. Ponikarov, I. M. Tsidil'kovskiĭ, and N. G. Shelushinina, Fiz. Tekh. Poluprovodn. **13**, 684 (1979) [Sov. Phys. Semicond. **13**, 402 (1979)].

[5]B. I. Shklovskiĭ and A. L. Éfros, Élektronnye svoĭstva legirovannykh poluprovodnikov (Electronic Properties of Doped Semiconductors), Nauka, Moscow, 1979.

[6]B. L. Gel'mont and M. I. D'yakonov, Zh. Eksp. Teor. Fiz. **62**, 713 (1972) [Sov. Phys. JETP **35**, 377 (1972)].

[7]F. R. Kusmartsez and É. I. Rashba, Pis'ma Zh. Eksp. Teor. Fiz. **37**, 106 (1983) [JETP Lett. **37**, 130 (1983)].

[8]B. I. Halperin and T. M. Rice, Rev. Mod. Phys. **40**, 775 (1968).

[9]A. A. Abrikosov, J. Low Temp. Phys. **18**, 185 (1975).

[10]V. I. Ivanov-Omskiĭ, N. N. Konstantinova, and K. P. Smekalova, Fiz. Tekh. Poluprovodn. **10**, 381 (1976) [Sov. Phys. Semicond. **10**, 227 (1976)].

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