Temperature dependence of the magnetoresistance in the regime of variable-range hopping conduction: results for doped CdTe

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A systematic detailed analysis of the temperature dependence of the magnetoresistance in the regime of variable-range hopping (VRH) conduction is performed for the first time on the basis of experimental data obtained for samples of doped CdTe crystals with different degrees of proximity to the metal–insulator transition over a broad range of magnetic fields, including regions with both negative and positive magnetoresistance. The analysis of both the position $H_{\min}$ of the minimum of the resistivity $\rho(H)$ and of $\rho(H_{\min})$ points to a decrease in the contribution of the negative magnetoresistance with decreasing temperature for samples which are not excessively close to the metal–insulator transition. A model which makes it possible to attribute such behavior to suppression of the negative magnetoresistance in the transition to conduction via states in the Coulomb gap is proposed, based on existing theoretical models of magnetoresistance in the VRH regime, which consider both the interference of different tunneling paths involving intermediate scattering centers and the deformation of the wave functions of the VRH sites. Various models of scattering centers are considered; the best agreement with experiment is achieved under the assumption that the main contribution is made by scatterers with energies in the effective VRH energy band. The results obtained are compared with the conclusions of previous theoretical and experimental investigations.

1. INTRODUCTION

Recently there has been heightened interest on the part of theoreticians and experimentalists in the problem of the magnetoresistance of unordered semiconductors in the region with variable-range hopping (VRH) conduction. This has been due, on the one hand, to the complexity and diversity of the corresponding physical picture, which is associated in different situations, particularly at different values of the magnetic field H, with different phenomena: quantum interference of the wave functions, which appears when the scattering of the tunneling carrier on intermediate sites is taken into account,[1] deformation of the wave functions of the impurity centers by a magnetic field (with or without scattering),[1] narrowing of the impurity band in a magnetic field,[2] and spin effects.[1] According to theoretical predictions, negative magnetoresistance should generally be observed in weak fields, and positive magnetoresistance should be observed in strong fields. Experimentally, both negative and positive magnetoresistance were observed in the VRH regime. In samples close to the metal–insulator transition [particularly in CdSe (Ref. 3) and in CdTe (Ref. 4)], negative magnetoresistance was always observed, but this cannot be said for materials far from this transition. In particular, it was found that the possibility of observing negative magnetoresistance in Ge depends on the degree of compensation.[5]

On the other hand, when magnetoresistance data are correctly interpreted, they can permit the determination of numerous parameters that characterize a given doped semiconductor and its proximity to the metal–insulator transition, such as the localization radius of impurity centers a, the density of states at the Fermi level ε_F, and the dielectric constant κ. This is possible, if the behavior of the density of states $g(\varepsilon)$ near the Fermi level, which determines the temperature dependence of the resistivity $\rho(T)$ in a given temperature range when $H=0$ is known. If $g(\varepsilon)=\text{const}$ holds, we have

$$\rho(T)=\rho_0\exp(T_0/T)^{1/4}, \quad T_0=\beta_0/g(\varepsilon_f)a^3, \tag{1}$$

If characteristic hopping occurs in the region of the Coulomb gap, $g(\varepsilon)=g_e\varepsilon^2$, then

$$\rho(T)=\rho_1\exp(T_1/T)^{1/2}, \quad T_1=\beta_1e^2/\kappa a\,. \tag{2}$$

Here β_0 and β_1 are numerical coefficients. In the preceding study[6] we investigated plots of $\rho(T)$ for doped CdTe(Cl) crystals with electron density $n\sim10^{17}$ cm^{-3} and different degrees of compensation K in the 0.4–4.2 K temperature range. It was shown that samples which are far from the metal–insulator transition exhibit crossover from law (1) to law (2) as the temperature is lowered. Samples which are very close to the metal–insulator transition exhibit only law (1), if the temperature dependence of the pre-exponential factor is included. This can be understood, if we take into account that, as the transition is approached, the Coulomb gap width decreases and, thus, law (2) is observed only at very low temperatures. It was shown that the parameters a and κ display appreciable divergence as the metal–insulator transition is approached.

In the present work the temperature dependence of the VRH conductivity was investigated in the 0.4–4 K temperature range on the same samples at various values of the magnetic field $H=0-6$ T. A model which explains the observed behavior was constructed on the basis of the existing theoretical ideas.

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TABLE I. Principal parameters of the samples.

No.	$n_{300\ K}$, cm^{-3}	a, Å	a', Å
1	$8 \cdot 10^{16}$	140	165
2	$9 \cdot 10^{16}$	220	240
3	$1.2 \cdot 10^{17}$	410	400

Here $n_{300\ K}$ is the electron density at 300 K found from Hall measurements; a is the localization radius found from the temperature dependence of the resistance based on Eq. (1), and a' is the localization radius found by analyzing the quadratic dependence of the positive magnetoresistance using Eqs. (13) and (14).

2. EXPERIMENT

The parameters of the samples evaluated from the plots of $\rho(T)$ at $H=0$ (see Ref. 6) are presented in Table I. The value of $n_{300\ K}$ (the electrons density at 300 K) is close to the critical density for the metal–insulator transition in uncompensated CdTe: $n_c=1.5\times10^{17}$ cm^{-3}. The total donor concentration evaluated from Hall measurements was equal to 2×10^{17}–5×10^{17} $cm^{-3}>n_c$, and the samples were on the insulator side of the transition owing to compensation.

Figures 1a, 1b, and 1c present plots of $\rho(H)$ for three samples at different temperatures. For $T>1$ K sample 3 displays only negative magnetoresistance over the entire range of magnetic fields. The other two samples display a transition from negative to positive magnetoresistance as H increases at the same temperatures. The value of the negative magnetoresistance at the value of H corresponding to the minimum of $\rho(H)/\rho(0)$ at first increases slowly as the temperature decreases to 1 K and then decreases rapidly for all the samples. The position of H_{min} for all the samples shifts toward weaker magnetic fields as the temperature decreases from 3 to 0.4 K, the value of H_{min} for sample 1 being equal to 0.4 T at $T=0.43$ K (see the insert in Fig. 1a). It may thus be concluded that the negative magnetoresistance vanishes (shifts toward weaker magnetic fields and decreases in magnitude) as the temperature is lowered. This disappearance of the negative magnetoresistance is most pronounced for the most strongly compensated sample (sample 1). At high temperatures a section for which the dependence of $\rho(H)$ is quadratic is observed at very weak magnetic fields and is replaced by a linear law as H increases (see the insert in Fig. 1b). However, at lower temperatures all the samples display negative magnetoresistance with linear behavior.

We now move on to the results for the region of higher magnetic fields. Plots of $\ln(\rho(H)/\rho(0))$ versus H^2 for sample 2 at various temperatures are shown in Fig. 2. It is seen that there is a clearly expressed section with a quadratic dependence of the positive magnetoresistance at $2T<H<4$ T, which shifts somewhat toward weaker magnetic fields as the temperature is lowered. For $H>3-4$ T the section with a quadratic dependence of the positive magnetoresistance is replaced by a section with positive magnetoresistance which is weakly dependent on H: at first the dependence is almost linear (see Fig. 1), and then the magnetoresistance is proportional to $H^{2/3}$. For $H>4$ T sample 3 displays a plateau as H varies at $T=0.43-1$ K (Fig. 1c). At higher temperatures this sample exhibits negative magnetoresistance over the entire range of magnetic fields, a second minimum of the negative magnetoresistance being observed for $H>4-5$ T.

3. THEORY

Here we focus our attention on the range of weak magnetic fields, where negative magnetoresistance and a transition to a quadratic dependence of the positive magnetoresistance are observed. As was first shown by Shklovskii and Spivak,[1] the negative magnetoresistance observed under the VRH regime at weak fields is caused by the interference

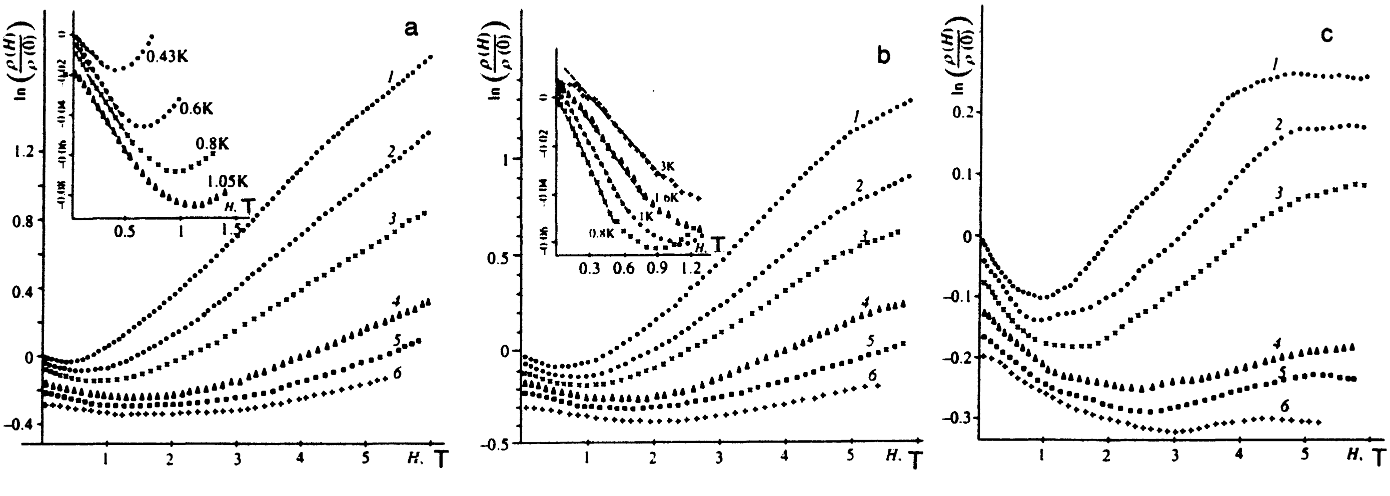

FIG. 1. Magnetoresistance of three samples of CdTe(Cl), whose parameters are indicated in Table I, for various temperatures: a) sample 1; b) sample 2; c) sample 3. The numbers of the curves correspond to 0.43 K (*1*), 0.6 K (*2*), 0.8 K (*3*), 1.3 K (*4*), 1.6 K (*5*), 3 K (*6*). The sections with a transition from negative to positive magnetoresistance for low temperatures are shown in detail in insert *a*. The initial sections of the negative magnetoresistance, where its quadratic character is displayed, are shown in detail in insert *b*.

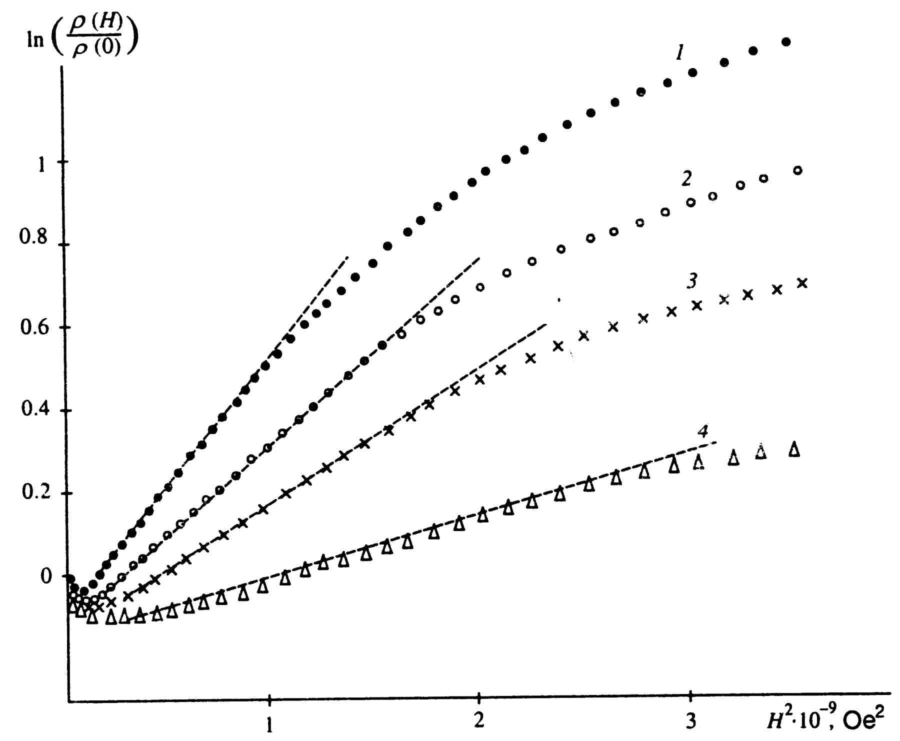

FIG. 2. Dependence of the resistivity of sample 2 on H^2 at 0.43 K (*1*), 0.6 K (*2*), 0.8 K (*3*), 1.6 K (*4*).

among the contributions to the hopping probability from different electron tunneling trajectories which include scattering events on intermediate impurities (see, for example, the review in Ref. 1). The fact is that the logarithms of the hopping probabilities, rather than the probabilities themselves, are averaged in the VRH regime, so that the configurations in which the contributions J_1 and J_2 of individual trajectories to the hopping probability amplitude compensate one another (due to the singularity of $\ln|J_1+J_2|$ when $J_1+J_2=0$ holds) are anomalously emphasized in the averaging over the impurity positions. Since in the absence of a magnetic field the probability amplitudes J_i are real, the application of a field [which results in the appearance of the phase factors $\exp(i\varphi)$, with $\varphi=2\pi\Phi/\Phi_0$, where Φ is the magnetic flux through the corresponding contour and $\Phi_0=\pi c\hbar/e$ is the quantum of flux] eliminates this compensation and thus increases the hopping probability and, accordingly, the conductivity.

Since numerical simulation methods were used for the most part in Ref. 1, there was no detailed analysis of the temperature-dependent behavior of the negative magnetoresistance (although it was pointed out, in particular, that the negative magnetoresistance for Mott conduction and conduction via states in the Coulomb gap can have different characters). We note that the corresponding temperature dependence was discussed in Refs. 7 and 8, but under some additional assumptions (we shall briefly discuss them later on), which, in our opinion, do not correspond to the situation in our experiment.

Therefore, a comparison of our experimental results with theory requires additional analysis, which we performed using the approach developed in Ref. 1. Let us consider the contribution of pairs of paths 1 and 2 joining sites 1 and 2, one of which includes scattering events on intermediate site 3, to the negative magnetoresistance:

$$\ln\frac{\rho(H)}{\rho(0)}=-\left\langle\int_{-\infty}^{\varepsilon_1-\Delta}d\varepsilon_3\int d\mathbf{r}_3 g(\varepsilon_3)\times\ln\left(1+J_1(J_1-J)\frac{\varphi^2}{J^2}\right)\right\rangle. \quad (3)$$

(We took into account that ε_1 must be greater than ε_2 for J_2 to be negative.) Here the angle brackets denote averaging over the energy of the first site ε_1; $\mathbf{r}_2$ and ε_2 are the coordinate and energy of the intermediate site; $J=J_1+J_2$, where $J_2=J_2(\varepsilon_3,\mathbf{r}_3)$. The parameter Δ takes into account the fact that the scattering center 3 (which is closer to site 1 than site 2) cannot have an energy very close to ε_1. Otherwise, the "resistor" corresponding to successive $1\rightarrow3$ and $3\rightarrow2$ hops would significantly shunt the contribution, which we are considering, of $1\rightarrow2$ hopping modified by scattering on site 3. According to Ref. 1, the condition $r_{13}+r_{32}<r+a$ (where $r\equiv r_{12}$ is the hopping distance) must hold in the situation under consideration. Hence we obtain the estimate $\Delta\geqslant W(r_{23}/r)$, where W is the characteristic energy band for VRH.

In analogy to Ref. 1, integration over $\mathbf{r}_3$ gives the volume of the region in which the scatterer must be found for a given $\mu(\varepsilon_3)$ in order that the condition $|J_2|=|J_1|$ could hold:

$$\ln\frac{\rho(H)}{\rho(0)}\sim-\left\langle\int_{-\infty}^{\varepsilon_1-\Delta}d\varepsilon_3 g(\varepsilon_3)\mu^2(\varepsilon_3)a\right\rangle|\varphi|, \quad (4)$$

where μ is the absolute value of the scattering amplitude and $|\varphi|\sim r(\mu a)^{1/2}H/\Phi_0$.

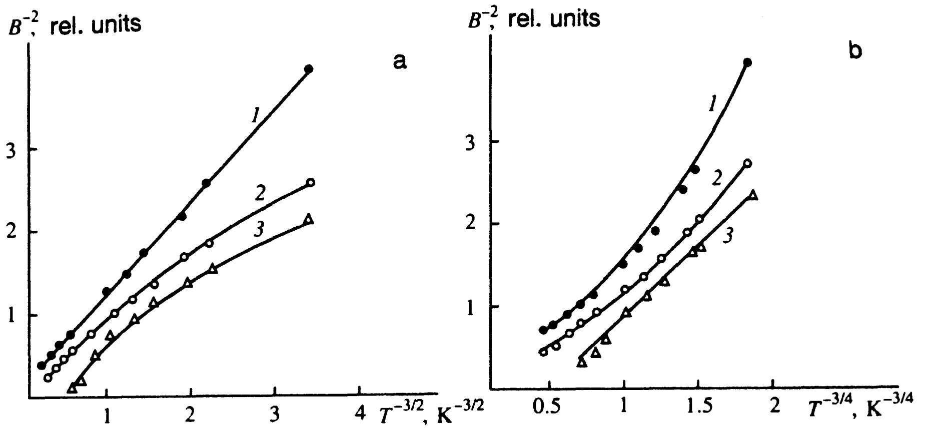

FIG. 3. Temperature dependences of B^{-2} corresponding to expressions (13) (a) and (14) (b). The numbers of the curves correspond to the numbers of the samples in Table I.

We note that the "three-site" approximation which we used presupposes the inequality

$$\gamma=\left\langle \int_{-\infty}^{\varepsilon_1-\Delta} d\varepsilon_3 g(\varepsilon_3)\mu^2(\varepsilon_3)a \right\rangle \ll 1, \tag{5}$$

which corresponds to the so-called "constant-sign" regime.

For μ we use the expression

$$\mu=\mu_0\left(\frac{\varepsilon_1}{\varepsilon_1-\varepsilon_3+\delta}\right)^{\beta}. \tag{6}$$

Here we have $\mu_0=\text{const}$, and β depends on the state of the site: $\beta=1$ holds for a free donor, while the values $\beta=1$ and $\beta=3$ are possible for an occupied site.[1] In (6) we noted that, on the basis of physical arguments, the result of the integration over $\mathbf{r}_3$ in (3) cannot exceed the effective volume corresponding to the value $\mu\sim r$, and we introduced the cut-off parameter δ, which corresponds to the requirement $\mu<r$, into (6):

$$\delta\sim|\varepsilon_1|\left(\frac{\mu_0}{r}\right)^{1/\beta}. \tag{7}$$

Note that an approximate expression for the parameter Δ introduced above can be written by using the requirement $r_{32}\leq\mu$ in (6) in the form $\Delta\sim(W\delta^{\beta}(r))^{1/(\beta+1)}$.

Other restrictions on μ are possible. For example, for neutral sites the quantity $r_0=e^2/\kappa(\varepsilon_1-\varepsilon_2)$, which characterizes the distribution of the charge in a scattering event, must not exceed the characteristic spatial scales (see, for example, Ref. 1). The distance to the nearest charged impurity N_D^{-3} should be regarded as such a scale. As a result, we obtain the estimate

$$\delta\sim\varepsilon_1 a_0 N_D^{-1/3}, \tag{8}$$

where a_0 is the localization radius for an isolated site.

Taking into account the different types of scattering by free (f) and occupied (o) sites we write (4) in the form

$$\ln\frac{\rho(H)}{\rho(0)}\sim(N_{\text{eff},f}\mu_{0,f}^{5/2}a^{3/2}+N_{\text{eff},o}\mu_{0,o}^{5/2}a^{3/2})\frac{H}{\Phi_0},$$

$$N_{\text{eff},f}=\int_0^{\max(0,\varepsilon_1-\Delta)} d\varepsilon\, g(\varepsilon)\left(\frac{\varepsilon_1}{\varepsilon_1-\varepsilon+\delta_f}\right)^{5/2},$$

$$N_{\text{eff},o}=\int_{-\infty}^{\min(0,\varepsilon_1-\Delta)} d\varepsilon\, g(\varepsilon)\left(\frac{\varepsilon_1}{\varepsilon_1-\varepsilon+\delta_o}\right)^{5\beta/2}. \tag{9}$$

Here we have noted that states located below the Fermi level are occupied for the most part. With consideration of (6), we have the following estimates for the integrals in (9):

$$N_{\text{eff},f}\sim g(W)\left(\frac{\varepsilon_F}{\max(\delta_f,(W\delta_f)^{1/2})}\right)^{5/2}\min(W,(W\delta_f)^{1/2}),$$

$$N_{\text{eff},o}\sim g(\max(W,\delta_0))\left(\frac{\varepsilon_F}{\max(\delta_0,(W\delta_o^{\beta})^{1/(\beta+1)})}\right)^{(5\beta-2)/2}. \tag{10}$$

As we know,[1] the positive magnetoresistance, which is associated with deformation of the wave functions of the sites in the magnetic field, begins to dominate in stronger magnetic fields. For VRH conduction in weak magnetic fields such that $\ln(\rho(H)/\rho(0))\ll1$ holds, the dependence of the positive magnetoresistance on the magnetic field is described by the expression[1]

$$\ln\frac{\rho(H)}{\rho(0)}=(H/\bar{B})^2, \tag{11}$$

where

$$B^2=\frac{\alpha c^2\hbar^2}{r^3ae^2} \tag{12}$$

is a parameter, which depends on the temperature, the localization radius, and the conduction mechanism [law (1) or (2)]:

$$B^2=\frac{c^2\hbar^2}{C_0e^2a^4}\left(\frac{T}{T_0}\right)^{3/4}, \tag{13}$$

$$B^2=\frac{c^2\hbar^2}{C_1e^2a^4}\left(\frac{T}{T_1}\right)^{3/2}. \tag{14}$$

Expression (13) corresponds to Mott's law, $C_0=0.0025$, and $\alpha\simeq400$, while expression (14) corresponds to conduction via states in the Coulomb gap, and two values are presented for C_1: 0.0015 ($\alpha\sim700$) and 0.0035 ($\alpha\sim300$) (see Fig. 3).

To compare the negative and positive magnetoresistance, it is convenient to express the negative magnetoresistance (9) in the form

$$\ln\frac{\rho(H)}{\rho(0)}=k\frac{H}{B}, \tag{15}$$

where B is specified by expressions (11) and (12),

$$k=k_f+k_o,\quad k_{f,o}=N_{\mathrm{eff},(f,o)}\alpha^{1/2}\mu_o^{5/2}\frac{a}{\pi r^{1/2}}. \tag{16}$$

Note that the value of B is equal to the critical magnetic field for the negative magnetoresistance in the "variable-sign" regime[1] to within the numerical factor $(\alpha\pi^2/12)^{1/2}$: $H_c\sim\Phi_0/r^{3/2}a^{1/2}$. Summing the two contributions we have

$$\ln\frac{\rho(H)}{\rho(0)}=-k\frac{H}{B}+\left(\frac{H}{B}\right)^2, \tag{17}$$

whence we at once obtain

$$H_{\min}=\frac{k}{2}B,\quad \ln\frac{\rho(H)}{\rho(0)}_{\min}=-\frac{k^2}{4}. \tag{18}$$

To analyze the temperature dependence of the magnetoresistance we note that

$$k_f\propto g(W)(\max(\delta_f,\sqrt{W\delta_f})^{-5/2}\min(W,\sqrt{W\delta_f})r^{-1/2},$$

$$k_o\propto g(\max(\delta_o(W\delta_o^{\beta})^{1/(\beta+1)}))^{-(5\beta-2)/2}r^{-1/2}. \tag{19}$$

The function $\delta(T)$ must be specified for further analysis. For free sites we assumed that δ_f is determined by the requirement $\mu<r$, i.e., relation (7) holds. Hence we have $\delta_f\propto r^{-1}$. In such a case for k_f we have

$$W<W_C:\ k_f\propto W^{5/4}r^{1/4}\propto T^{1/2}\ (\delta_f<W),$$

$$k_f\propto W^2 r\propto T^{1/2} \tag{20}$$

(here W_C is the Coulomb gap width; we took into account that in the corresponding regime $W\propto r^{-1}\propto T^{1/2}$ holds),

$$W>W_C:\ k_f\propto W^{-3/4}\delta^{-3/4}r^{-1/2}\propto T^{-1/4}\ (\delta_f<W),$$

$$k_f\propto Wr^2\propto T^{1/4}. \tag{21}$$

Under the same assumption regarding the nature of δ_0, for $\beta=3$ we have $\delta_0\propto r^{-1/3}$, and for k_0 we obtain

$$W>W_C:\ k_o\propto W^{-13/8}r^{9/8}\propto T^{-5/4}\ (\delta_o<W),$$

$$k_o\propto r^{10/6}\propto T^{-5/12}(\delta_o>W),$$

$$W<W_C:\ k_o\propto W^{3/8}r^{9/8}\propto T^{-3/8}\ (W>\delta_o),$$

$$k_o\propto\delta_o^{-9/2}r^{-1/2}\propto T^{-2/3}(W<\delta_o). \tag{22}$$

If it is assumed that δ_0 is controlled by the requirement $r_0<N_D^{-1/3}$ and, thus, δ_0 = const, we have

$$W>W_C:\ k_o\propto r^{-1/2}\propto T^{1/8},$$

$$W<W_C:\ k_o\propto r^{-1/2}\propto T^{1/4}\ (W<\delta_o),$$

$$k_o\propto W^2r^{-1/2}\propto T^{5/4}(W>\delta_o). \tag{23}$$

We note that if the value of β in (6) for occupied sites is equal to unity, as it is for free sites, we have [under assumption (7)]

$$\delta_o\ll W<W_C:\ k_o\sim g(W)\left(\frac{\varepsilon_F}{\sqrt{W\delta_o}}\right)^{3/2}r^{-1/2}\propto T^{1/2} \tag{24}$$

(i.e., just as for free sites). However, when δ_0 is not excessively small, the competition between the increase in the denominator in the corresponding integrand in (9) when ε increases (which corresponds to the "singular" contribution discussed above) and the increase in $g(\varepsilon)\propto\varepsilon^2$ is significant, and the contribution of the energies $\varepsilon\geqslant W_C$ can become significant as a result. It is not difficult to see that the corresponding contribution can be neglected only if

$$\frac{g(W)}{g(W_C)}\left(\frac{\sqrt{W\delta_o}}{W_C}\right)^{3/2}\sim\left(\frac{W}{W_C}\right)^{1/2}\left(\frac{W}{\delta_o}\right)^{3/4}>1.$$

Accordingly, for large δ_o we have

$$\delta_o<W_C:\ k_o\propto g(W_C)\frac{\varepsilon_F^{5/2}}{W_C^{3/2}r^{1/2}}\propto T^{1/4},$$

$$W_C<\delta_o<W:\ k_o\propto(W\delta_o)^{-3/4}r^{-1/2}\propto T^{-5/8},$$

$$\delta_o>W>W_C:\ k_o\propto\delta_o^{-3/2}r^{-1/2}\propto T^{1/4}. \tag{25}$$

The estimates obtained are summarized in Table II.

It is not difficult to see that expression (16) for the parameter k incorporating of is distinguished from expression (5) for the parameter γ, which characterizes the "sign regime" (see Ref. 1), by the factor $(\alpha^{1/2}/\pi)(\mu/r)^{1/2}$ (in the integrand), which, under assumption (7), leads to the relation $k/\gamma\sim\alpha^{1/2}/\pi\sim 7$. Thus, the temperature dependence of k attests to a corresponding dependence of γ and, thus, can cause a "sign transition" as the temperature varies. In particular, according to (20), under the Coulomb gap regime a transition from the "variable-sign" regime to the "constant-sign" regime can be expected as the temperature is lowered. Such a possibility was pointed out in Ref. 1.

Let us now compare the estimates presented with the calculations performed in Refs. 7 and 8.

The calculations in Ref. 7 were performed under the assumption that the energy of the intermediate site ε_2 must be outside of the band of energies W of the sites mediating hopping transfer. In addition, the pre-exponential dependence of the probability amplitude J_2 on the coordinate of scattering center 3 was not taken into account. In our opinion, this restriction on the value of ε_3 is excessively rigid. The calculations presented above reflect the fact that the permissible closeness of the energies of sites 1 and 3 depends on the relationship between the distances r_{12} and r_{13}, i.e., on the coordinate of site 3.

The possible role of imaginary additions to the energies of the sites, which are caused by the finite nature of the lifetimes τ of the corresponding states and result in a nonzero "phase shift" even in the absence of a magnetic field, was analyzed in Ref. 8. It was shown, in particular, that this factor can result in the replacement of a linear dependence of the negative magnetoresistance by a quadratic dependence and even in a change in the sign (to a positive sign). However, as can be seen from the calculations in Ref. 8, this behavior should be displayed, if the phase shift of the type indicated $\propto\hbar/\tau(\varepsilon_1-\varepsilon_i)$ exceeds the shift φ caused by the

TABLE II. Behavior of k for various hypotheses regarding the nature of the scattering centers.

	$\delta < W < W_C$	$W < \delta < W_C$	$W_C < W < \delta$	$W_C, \delta < W$
Free sites	$\propto T^{1/2}$	$\propto T^{1/2}$	$\propto T^{1/4}$	$\propto T^{-5/8}$
Occupied sites $\beta = 3$	$\propto T^{-3/8}$	$\propto T^{-1/2}$	$\propto T^{-5/12}$	$\propto T^{-5/4}$
$\beta = 3$, $\delta = \text{const}$	$\propto T^{5/4}$	$\propto T^{1/4}$	$\propto T^{1/8}$	$\propto T^{1/8}$
$\beta = 1$,	$\propto T^{1/2}$	$\propto T^{1/4}$	$\propto T^{-1/4}$	$\propto T^{-5/8}$

magnetic field. Since the values of $\hbar/\tau$ are smaller than the characteristic energies of the problem even for sites which whose energy is far from ε_F, ordinary negative magnetoresistance[1] should be observed, in our opinion, for values of φ that are not too small. However, the mechanism in Ref. 8 can mediate the transition to a quadratic dependence of the negative magnetoresistance as $H \rightarrow 0$ and can thus compete with the mechanism proposed in Ref. 1.

4. DISCUSSION OF RESULTS

Utilizing the theoretical arguments above, we first of all analyze the region of negative magnetoresistance and the transition to positive magnetoresistance with a quadratic dependence, particularly the temperature dependence of the following parameters: $H_{\min}$, $\ln(\rho(H_{\min})/\rho(0))$, and $d\rho/dH$. The corresponding plots are presented in Figs. 4a, 4b, and 4c.

Before proceeding to a more detailed analysis of these plots, we note that the theoretical predictions obtained under different assumptions regarding the nature of the scattering exhibit some common features. More specifically, a decrease in the value of k with decreasing temperature is generally displayed in the Coulomb gap regime, while a decrease in k with *increasing* temperature is observed in the Mott conduction regime (one exception is the case of occupied sites with $\beta=3$; however, even for them the transition to the Coulomb gap regime with decreasing T is associated with weakening of the increase in k). Accordingly, it may be expected that the transition from VRH conduction of the Mott type to VRH conduction via states in the Coulomb gap should be accompanied by a change in the character of the temperature dependence of the negative magnetoresistance from an increase

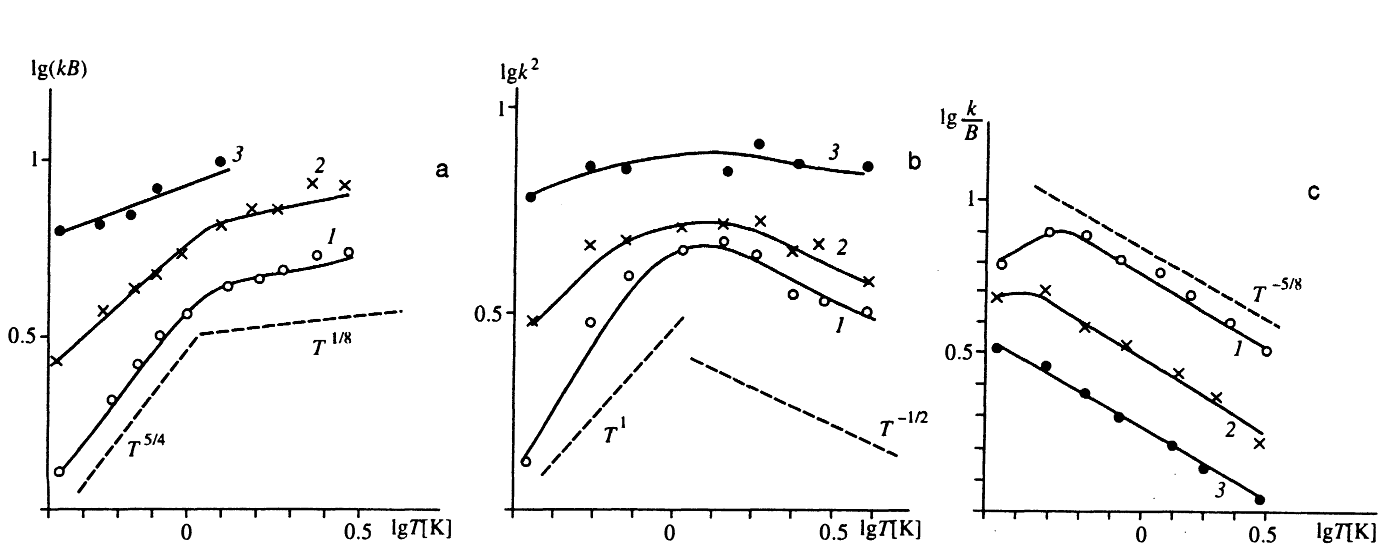

FIG. 4. Temperature dependence of several parameters determined from the magnetoresistance curves: a) $H_{\min} \sim kB$; b) $\ln(\rho(H)/\rho(0))_{\min} \sim k^2$; c) $\Delta\rho(H)/H\rho(0) \sim k/B$. The theoretical predictions for various limiting cases are represented by dashed lines.

in the negative magnetoresistance with decreasing temperature to a decrease.

As we see, the experimental curves for samples 1 and 2 [whose temperature dependence of $\rho(T)$ exhibits a transition from conduction of the Mott type to conduction via states in the Coulomb gap[6] at $T=1$ K] do, in fact, reveal a significant change in the temperature dependence at temperatures on the order of the temperature for this crossover, which is in qualitative agreement with the predictions of the theory. We proceed to a more detailed discussion.

According to Fig. 4a, an abrupt change in the temperature dependence of $H_{\min}(T)$ is observed for samples 1 and 2 as the temperature is lowered. In the low-temperature range $T<1$ K in these samples $H_{\min}(T)$ is close to a $T^{5/4}$ law. Such behavior is consistent with (18), if expression (20) is used for k, i.e., under the assumption that we are dealing with VRH conduction via states in the Coulomb gap and free sites predominate in the scattering. In fact, in this case we have $H_{\min}\propto k_f B \propto T^{3/4}T^{1/2}=T^{5/4}$. This same law is also expected for scattering on occupied sites under assumptions (24).

At high temperatures these samples exhibit a considerably weaker increase in $H_{\min}$ with increasing temperature, which approximates a $T^{1/8}$ law. It is not difficult to see that in general the theory predicts an even sharper change in the temperature dependence ($H_{\min}\propto T^{-5/8}T^{3/8}=T^{-2/8}$) for scattering on free sites in the corresponding temperature range $(W_C,\delta)<W$. The observed behavior is described well by the expression for occupied sites with $\beta=1$ and $W_C<W<\delta$ ($H_{\min}\propto T^{-1/4}T^{3/8}=T^{1/8}$). However, when this relationship exists between the parameters, an appreciable manifestation of the contribution of the states with $\varepsilon\sim W_C$ to the scattering [see Eq. (25)], which decreases slowly with decreasing temperature, would be expected for the occupied sites (this is not consistent with the data for the low-temperature region).

As for sample 3, at sufficiently high temperature it does not display any pronounced minimum of the resistivity, which is nearly saturated in sufficiently strong fields. In our opinion, this may be evidence either of the "variable-sign" regime or, in any case, of the closeness of the samples to the "sign transition."[1] When the temperature is lowered, however, positive magnetoresistance and, accordingly, a minimum of $\rho(H)$, whose position shifts slowly with decreasing temperature, begin to appear. As we saw above, the latter is characteristic of Mott conduction.

Let us now turn to the value of the resistance at the minimum (Fig. 4), which can be expressed directly in terms of k [see Eq. (18)] and, thus, characterizes the magnitude of the negative magnetoresistance. At high temperatures samples 1 and 2 display an increase in the negative magnetoresistance with decreasing temperature, as the theory predicts for the region corresponding to Mott's law. However, the observed behavior is close to a $T^{-1/2}$ law, while the theory for both free and occupied ($\beta=1$) sites presents a more rapid increase in the negative magnetoresistance with decreasing $T\propto T^{-5/4}$ for the highest temperature range $(W_C,\delta)<W$. As in the case of $H_{\min}$ in the corresponding temperature range, optimal agreement is achieved here for the occupied sites in the range $W_C<W<\delta$; however, problems arise here in attempting to quantitatively explain the behavior in the low-temperature region.

At $T<1$ K both samples display a considerable decrease in the negative magnetoresistance as T is lowered. This, in turn, is consistent with the theoretical prediction [see Eq. (20) and (24)] for the Coulomb gap regime in the case of scattering on free and occupied sites ($\beta=1$), $k^2\propto T$.

Sample 3 does not display noticeable suppression of the negative magnetoresistance as the temperature is lowered, in agreement with the data on the temperature dependence of the conductivity in Ref. 6, where only Mott conduction was observed over the entire temperature range. The value of the negative magnetoresistance at the minimum scarcely varies over the entire temperature range where the minimum is observed. In general, this is not consistent with the predictions of the model under consideration under the assumptions that we previously used. In our opinion, this may be due to the closeness of $H_{\min}$ to H_c, which precludes the use of the linear approximation for the negative magnetoresistance.

An analysis of the plots of the temperature dependence of the slopes of the linear segments of the negative magnetoresistance reveals that for $T>0.8$ K all the samples obey a nearly $T^{-0.6}$ to $T^{-0.7}$ law. Since $d\rho(H)/dH=k/B$ (15), this law is somewhat weaker than that predicted by evaluations for Mott's law in the range corresponding to the last column in Table II ($\propto T^{-1}$). Note that samples 1 and 2 exhibit appreciable weakening of this dependence at temperatures below 0.8 K, in agreement with the picture of the transition to the regime with conduction via states in the Coulomb gap [see Eq. (20)]: $k/B\propto T^{1/2}T^{-3/4}=T^{-1/4}$. Thus, the plots of the temperature dependence of the slopes of the linear segments of the negative magnetoresistance also attest to a decrease in the latter in the regime with conduction via states in the Coulomb gap. However, in our opinion, the behavior of $\rho(H_{\min})$ is more informative in this respect.

We note that the slight quantitative disparities between the theoretical evaluations and the observed behavior can be attributed to the comparative narrowness of the temperature range investigated, which precludes revealing the asymptotic behavior of the quantities investigated. It is, however, noteworthy that, as can be seen, the agreement with experiment in the Mott region for both free and occupied sites with $\beta=1$ and $(W_C,\delta)<W$ would be just as good as for $\beta=1$ and $W<\delta$, if there were no restriction on the closeness of the energy of the scattering center to ε_1 [this would correspond to $\Delta=0$ in Eq. (9)], since in that case we would have $k\propto T^{-1/4}$ in the situations indicated.

At the same time, we wish to note that, as follows from the theoretical evaluations, the observed sharp changes in the temperature dependences cannot be explained under any of the hypotheses regarding the scattering mechanisms considered, if it is assumed that the entire temperature range investigated corresponds to a single regime of VRH conduction, for example, the regime of conduction via states in the Coulomb gap.

We also wish to stress that, in our opinion, an investigation of the temperature dependence of the minimum of the negative magnetoresistance can be more productive from the standpoint of studying the details of VRH conduction (including the crossover indicated) than a direct study of the temperature dependence of ρ, since the negative magnetoresistance is related, in principle, to the pre-exponential factors and is not subject to an exponential temperature dependence.

In particular, as follows from our investigations, the temperature-dependent behavior of the negative magnetoresistance is very sensitive to the characteristics of the scatterers (in contrast to the existing theories). For example, scattering on occupied scatterers, which is treated in analogy to scattering on a hydrogen atom ($\beta=3$), produces a picture which differs qualitatively from the experimentally observed picture. In our opinion, this conclusion raises interest in a more detailed investigation of subbarrier scattering processes at sites of different types.

As for the region of very weak magnetic fields, it was pointed out above that a pronounced section with a quadratic dependence of the negative magnetoresistance is observed in it at high temperatures (see Fig. 2) and that it nearly vanishes when the temperature is lowered. Such behavior is consistent with the predictions in Ref. 1, which attribute the quadratic dependence of the negative magnetoresistance to the lower bound placed on the probability amplitude J [see Eq. (3)]: $|J|>\exp(-r/a)$, which, as is seen from (3), causes the linear $\rho(H)$ law to become quadratic for $|\varphi|\sim Hr^{3/2}A^{1/2}/\Phi_0<\exp(-r/a)$. In fact, according to the present evaluation the region of the quadratic dependence of the negative magnetoresistance narrows exponentially as $T\rightarrow 0$. On the other hand, in our opinion, the experimental results do not display the mechanism in Ref. 8, under which the quadratic dependence of the negative magnetoresistance should be enhanced as the temperature is lowered.

Let us now proceed to an analysis of the region of positive magnetoresistance.

Figure 3 shows plots of the temperature dependence of the slope of the quadratic positive magnetoresistance (B^{-2}) recorded in the 0.43–3 K range. It is seen that the dependence for sample 1 is described well by expression (14) over the entire temperature range, that the dependence for sample 3 is described well by expression (13), and that sample 2 exhibits intermediate behavior. The data on the temperature dependence of the conductivity for sample 2 and sample 1 attest to a transition from Mott conduction to conduction via states in the Coulomb gap when the temperature is lowered at $T<1-3$ K. This transition occurs at higher temperatures for sample 1 than for sample 2. In the case of sample 3, only Mott conduction was observed in the 0.43–3 K temperature range. This also corresponds to the data on the quadratic dependence of the positive magnetoresistance. The values of the localization radius evaluated from B using expressions (13) and (14) are presented in Table 1. They are in good agreement with the values of a obtained from T_0 [see expression (1)].

At stronger magnetic fields, all the samples display a pronounced deviation of the dependence of the positive magnetoresistance $\rho(H)$ away from the quadratic law toward a weaker dependence (Figs. 1 and 2). As was noted in Refs. 1 and 9, such behavior is attributable to the role of the intermediate scatterers: smallness of the distance between successive scatterers in comparison with r ensures lowering of the "magnetic barrier" (caused by deformation of the wave functions in the magnetic field) and, accordingly, an increase in the hopping probability (i.e., lowering of the resistivity) in comparison with the case of no scatterers (11). According to the theory in Ref. 9, as H increases there should be successive changes in the laws governing the positive magnetoresistance: $\propto H^2\rightarrow H^{5/4}\rightarrow H^{2/3}\rightarrow H^{1/4}$. Unfortunately, the comparatively narrow range of variation of H precludes performing a quantitative analysis of the corresponding experimental behavior.

As for sample 3 (which does not display positive magnetoresistance at high temperatures), at low temperatures where positive magnetoresistance is observed the latter practically reaches saturation in strong fields. In our opinion, such behavior occurs because this sample violates the inequality $N\mu^2a<1$, where $N\sim N_D$ and $\mu\sim a$ are the concentration and amplitude of the scattering for "constant-sign" scattering centers (which may be free donors with $\varepsilon_i>\varepsilon_F+W$). When this inequality holds, the inclusion of additional scattering centers not only lowers the "magnetic barrier," but also causes an increase in the effective tunneling path; optimization of the number of scatterers leads to the behavior of $\rho(H)$ indicated above. Violation of the corresponding inequality eliminates the effect associated with an increase in the tunneling path, so that intermediate scattering completely suppresses the subsequent increase in the magnetoresistance with increasing H.

As for the high-temperature range, sample 3 displays a new section with negative magnetoresistance, rather than positive magnetoresistance. In our opinion, this may be caused by the mechanism proposed in Ref. 2. The latter is attributed to alternation of the form of the impurity band in strong fields due to an increase in the degree of localization of the wave functions. More specifically, the shift toward the "dielectric limit" with respect to the metal–insulator transition as the field increases results in suppression of the "tail" of the density of states and, thus, in an increase in the density of states at the Fermi level. This, in turn, causes an increase in conductivity.

5. CONCLUSIONS

Although the conception of negative magnetoresistance in the hopping conduction regime has been adequately developed, the interpretation of the available experimental data is still not completely clear. In particular, in several experimental studies negative magnetoresistance was not detected at all over a broad temperature range (see, for example, Ref. 5). On the other hand, an increase in the negative magnetoresistance with decreasing temperature was reported in other papers (see, for example, Ref. 3). We believe that the results obtained here clarify the question under consideration to a certain extent. In our opinion, this applies to the observation of a nonmonotonic dependence of the negative magnetoresistance on the temperature and its suppression under the regime of conduction via states in the Coulomb gap.

The observed behavior can be explained under the assumption that scattering centers with energies in the characteristic energy band for VRH conduction, on which the scattering is close to resonance, play a decisive role in shaping the negative magnetoresistance. Just their contribution provides for suppression of the negative magnetoresistance under the regime of conduction via states in the Coulomb gap.

At the same time, it should be noted that, as the theoretical evaluations show, the situation investigated includes various possibilities associated with the possible diversity of theparameters of the scattering centers. This can account for the definite disparities in the data on the behavior of the negative magnetoresistance for different materials.

The results which we obtained are consistent with the experimental data in Ref. 10 for samples of CdSe, which exhibit an increase in the slope of the linear segment of the negative magnetoresistance proportional to $T^{-\nu}$, as the temperature is lowered where $\nu \sim 0.7$, and very weak displacement of the minimum as the temperature varies. In our opinion, this attests to VRH conduction of the Mott type in these samples, which are in close proximity to the metal–insulator transition ($n/n_c \sim 0.9$). Our sample which is closest to that transition displays similar behavior. We also wish to stress the closeness of all the parameters of the materials which we investigated and to those of the materials in Ref. 10.

Finally, we note that the plots of the temperature dependence of $H_{\min}$ and $\Delta\rho(H_{\min})$ for samples 1 and 2 exhibit a crossover from conduction of the Mott type to conduction via states in the Coulomb gap, which was previously observed in the temperature dependence of $\rho(T)$.

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[1] B. I. Shklovskii and B. Z. Spivak, in *Hopping Transport in Solids*, edited by M. Pollak and B. Shklovskii, Elsevier, 1991, p. 271.
[2] M. E. Raikh, J. Czingon, Qiu-Yi Ye, F. Koch *et al.*, Phys. Rev. B **45**, 6015 (1992).
[3] Youzhu Zhang, Peihua Dai, and M. P. Sarachik, Phys. Rev. B **45**, 9473 (1992).
[4] E. N. Arkad'eva, O. A. Matveev, and Yu. V. Rud', Fiz. Tekh. Poluprovodn. **2**, 830 (1968) [Sov. Phys. Semicond. **2**, 691 (1968)].
[5] A. N. Ionov and I. S. Shlimak, in *Hopping Transport in Solids*, edited by M. Pollak and B. Shklovskii, Elsevier, 1991, p. 397; A. N. Ionov, R. Renztch, and A. Jilevsky, in *Hopping and Related Phenomena 5, Proceedings of the 5th International Conference, Sept. 1993*, edited by C. J. Adkins and J. A. Meluness, World Science, 1994, p. 271.
[6] N. V. Agrinskaya and V. I. Kozub, Zh. Éksp. Teor. Fiz., **106**, 848 (1994) [J. Exp. Theor. Phys. **79**, 466 (1994)].
[7] W. Schirmacher, Phys. Rev. B **41**, 2461 (1990).
[8] O. Entin-Wohlman, Y. Levinson, and A. G. Aronov, Phys. Rev. B **49**, 5165 (1994).
[9] B. I. Shklovskiĭ, Fiz. Tekh. Poluprovodn. **17**, 2055 (1983) [Sov. Phys. Semicond. **17**, 1311 (1983)].
[10] Y. Zhang, P. Dai, and M. P. Sarachik, in *Proceedings of the 21st International Conference on the Physics of Semiconductors, China, 1992*, World Science, 1992, p. 265.

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