

Study of compensation in insulating and metallic *n*-type CdSe using transport measurements

M. Levy, A. Roy, and M. P. Sarachik

Department of Physics, City College of the City University of New York, New York, New York 10031

L. L. Isaacs

Department of Chemical Engineering, City College of the City University of New York, New York, New York 10031

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The resistivity and the Hall coefficient of indium-doped cadmium selenide with carrier concentrations spanning the insulator-to-metal transition have been measured as a function of temperature. We demonstrate that use of the Hall mobility deduced from these data and careful analysis and application of recent theory yield an estimate of the degree of compensation, $K = N_A/N_D$, for metallic as well as insulating material. Combining these results with Hall coefficient measurements at room temperature, one can then estimate both the number of donors, N_D , and acceptors, N_A .

I. INTRODUCTION

The transition from insulating to metallic behavior which occurs in semiconductors as the dopant concentration is increased has been the subject of numerous studies in recent years. Attention has focussed largely on doped silicon and germanium, which have the important advantage that the dopant levels can be well controlled and the concentration of unwanted impurities can be kept very small. These materials have indirect fundamental band gaps, however, a fact which may introduce complications in the interpretation of results and which also makes some interesting measurements, such as Faraday rotation, very difficult to perform and to analyze. On the other hand, direct-band-gap semiconductors such as CdS and CdSe are much more difficult to prepare cleanly and controllably. In addition to having non-negligible concentrations of unintended impurities, some degree of self-compensation is unavoidable. In order to shed further light on the metal-insulator transition, useful studies of these materials require full and careful characterization using a variety of different experimental probes. The aim is to obtain information regarding impurity content, the energy-level diagram including impurity levels, impurity bands and, if possible, the degree of compensation.

In this paper, we demonstrate that a careful analysis of Hall coefficient and resistivity data obtained for *n*-type CdSe with indium dopant concentrations spanning the metal-insulator transition can be used to estimate the degree of compensation, and thus both the numbers of donors and of acceptors. Although this has been done for semiconductors on the insulating side of the *M-I* transition ($n < n_c$), albeit not always with great care, we show that application of recent theory yields similar information regarding the compensation for metallic samples ($n > n_c$).

In the following, we briefly describe our experimental methods, and based on theory and on preliminary data taken down to 1.2 K, we make an estimate of the critical concentration n_c . We discuss the overall features of the Hall coefficient and resistivity data; we attribute the ex-

perimentally observed transport at high temperatures to carriers activated into the conduction band, and we argue that the behavior at intermediate temperature is very likely associated with impurity band conduction. Using the temperature-dependent mobility deduced by combining the results of the resistivity and Hall coefficient measurements, we then show in detail using available recent theory for the insulating, intermediate and metallic cases, how to estimate the compensation for samples on the metallic as well as the insulating side of the transition.

II. EXPERIMENTAL PROCEDURE

Samples of *n*-type CdSe doped with indium were obtained from two different sources, as specified in Table I. Five of the samples, of which four are on the insulating side of the transition, were purchased from Cleveland Crystals; the remaining samples, all metallic, were provided by the Institute of Physics, Polish Academy of Sciences in Warsaw. For ease of identification the prefixes *I* and *M* denote insulating and metallic, respectively. CdSe is self-compensating so that some degree of compensation is unavoidable. The concentrations listed in Table I were determined from the room-temperature value of the Hall coefficient, making the usual assumption that the ratio of Hall mobility to drift mobility is unity, that is, $r_H = \mu_H/\mu_D = 1$. Based on measurements of the temperature dependence of the Hall coefficient, we estimate that all but at most 10% of the carriers have been activated into extended states at room temperature. Based on our estimate of $3.0 \times 10^{17} \text{ cm}^{-3}$ for the critical concentration in CdSe, four of the samples, *I1* to *I4*, are insulating, and the remaining are on the metallic side of the transition.

Samples were cut with their faces perpendicular to the *c* axis to a size of approximately $3 \times 4 \times 0.8 \text{ mm}^3$. Using the van der Pauw¹ method, the resistivity and the Hall coefficient were determined both at room temperature, and in a cold-finger cryostat between 8 and 80 K.

In addition, data were obtained down to 1.25 K for sample *I4*, with a room-temperature carrier concentration $n_0 = 2.4 \times 10^{17} \text{ cm}^{-3}$, and up to 200 K for sample

TABLE I. Room-temperature resistivity ρ , carrier concentration n , deduced from room-temperature Hall coefficient, and sample source. The prefixes *I* and *M* denote insulating and metallic materials; the symbols CC and PAS refer to Cleveland Crystals and to the Institute of Physics of the Polish Academy of Sciences, respectively. The sample labeled *I1* represents two contiguous pieces cut from the same CdSe crystal. Data on Fig. 2 for sample *I1* correspond to one of those pieces for high temperatures and the other for low temperatures.

Sample	n (10^{17} cm^{-3})	ρ ($\Omega \text{ cm}$)	Source
<i>I1</i>	1.0	0.090	CC
<i>I2</i>	1.2	0.078	CC
<i>I3</i>	1.7	0.059	CC
<i>I4</i>	2.4	0.039	CC
<i>M1</i>	3.7	0.032	PAS
<i>M2</i>	5.0	0.022	PAS
<i>M3</i>	13.6	0.009	CC
<i>M4</i>	18.9	0.007	PAS

M2, with $n_0 = 5 \times 10^{17} \text{ cm}^{-3}$. Hall coefficient measurements were obtained in magnetic fields up to 6 kG. Within a given run, the resistivity and the Hall coefficient were determined to 0.5% and 3%, respectively; for both measurements, the reproducibility from run to run was 3–4 %.

III. RESULTS AND DISCUSSION

A. General features

Use of the Mott criterion,²

$$N_c^{1/3} a_H = 0.26 \pm 0.05, \quad (1)$$

where a_H is the effective Bohr radius of the impurity center, yields a critical concentration $N_c = (3.1 \pm 1.4) \times 10^{17} \text{ cm}^{-3}$ for uncompensated CdSe. Hirsch and Holcomb³ studied the effect of compensation on the critical carrier concentration n_c in Si:P,B. Their results agree qualitatively with previous studies in compensated Ge, and show an increase of n_c with compensation K . They find that the Ge data can be fit roughly by the form $n_c = N_c(K=0)/(1-K)$, whereas their Si data approximately follows the form $n_c = N_c(K=0)/(1-K)^{1/2}$. For typical values of the compensation in our samples, either of these two forms would give corrections which are well within the error bars of our estimate for N_c for CdSe obtained from the Mott criterion.

Figure 1 shows preliminary results obtained for (the logarithm of) the resistivity as a function of $T^{-1/4}$ down to 1.2 K for sample *I4*. (Data on an extensive series of samples near the transition, and a full discussion of results, will be published in a forthcoming article.) The behavior shown in Fig. 1 is consistent with Mott variable range hopping; we have recently found similar behavior for a slightly more concentrated ($2.8 \times 10^{17} \text{ cm}^{-3}$) sample, indicating that (compensated) *n*-type CdSe is probably insulating up to this concentration. On the other hand, sample *M1* with $3.7 \times 10^{17} \text{ cm}^{-3}$ exhibits metallic characteristics, so that we can place the critical concen-

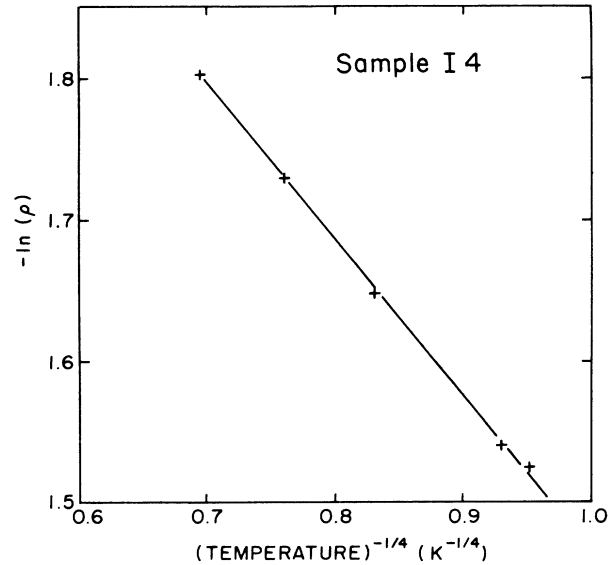


FIG. 1. Logarithm of the resistivity as a function of $T^{-1/4}$ for insulating sample *I4*. The straight line is drawn as a guide to the eye, and indicates Mott hopping conductivity occurs in this range of temperature.

tration at $(3.2 \pm 0.4) \times 10^{17} \text{ cm}^{-3}$ for compensations between 30% and 50%.

The conductivity of insulating doped semiconductors over a wider range of temperature is given by the well-known expression:⁴

$$\begin{aligned} \sigma = & \sigma_1 \exp(-\epsilon_1/kT) + \sigma_2 \exp(-\epsilon_2/kT) \\ & + \sigma_3 \exp(-\epsilon_3/kT). \end{aligned} \quad (2)$$

The first term refers to activation of electrons to the conduction band, the second describes activation to the mobility edge in an impurity D^- band of double occupancy states and the last term, which becomes dominant at low temperatures in compensated materials refers to Miller-Abrahams (fixed range) hopping. At still lower temperatures one expects to find Mott variable range hopping conduction as in Fig. 1. The prefactor σ_2 of the second term is the Mott minimum metallic conductivity

$$\sigma_{\min} = 0.026e^2 / \hbar d_c, \quad (3)$$

where d_c is the average separation between impurities at the critical concentration n_c .

It is apparent that for the four insulating samples shown in Fig. 2, there are two distinct temperature ranges in which the resistivity is characterized by different activation energies. The slopes of the straight lines observed at low values of $1/T$ (high temperatures) yield the parameter ϵ_1 , listed for samples *I1* and *I2* in Table II, which we associate with activation to the conduction band. Fits of Eq. (2) to the straight-line behavior at high values of $1/T$ (lower temperature) give for these same samples the prefactors σ_2 and activation energies ϵ_2 listed in Table II which we ascribe to activation to double occupancy states above the mobility edge in an impurity band. We base this claim on the fact that the experimentally determined prefactor σ_2 of Eq. (2) is consistent with

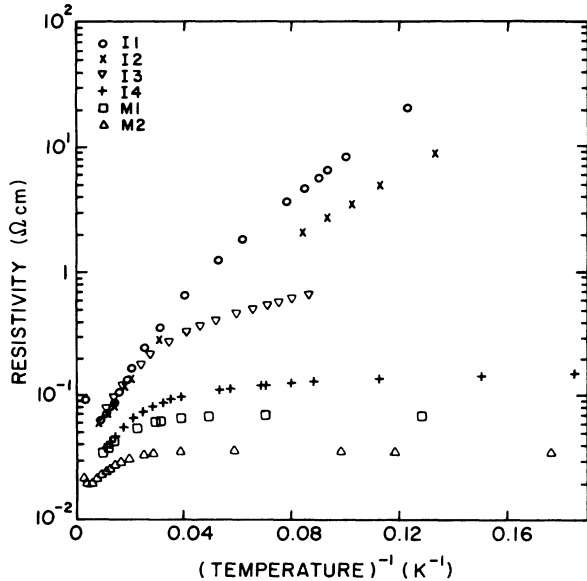


FIG. 2. Resistivity as a function of inverse temperature of n -type CdSe spanning the metal-insulator transition. The prefixes I and M denote insulating and metallic samples, respectively.

theoretical predictions for the value of Mott's minimum metallic conductivity in CdSe, and that compensation levels are low enough, as we shall show later, that a D^- band still exists which can support doubly occupied electron states. At the critical concentration of CdSe the average distance d_c between impurity centers, Eq. (3) yields a Mott minimum metallic conductivity σ_{\min} of about $690 (\Omega \text{ m})^{-1}$ for uncompensated material. This number must be corrected for the presence of compensation, which reduces the interimpurity separation d_c and shifts the critical concentration n_c upwards.^{2,5} An estimate of such a correction for typical compensations in our samples yields an approximate value of about $800 (\Omega \text{ m})^{-1}$. For compensated samples, however, Fritzsche² has argued that a correct calculation of the statistics of correlated electrons yields a Fermi energy which is a decreasing function of temperature, with the consequence that the apparent (measured) prefactor can be substantially reduced for sufficiently large compensation. At $K=0.5$, for example, this effect reduces σ_{\min} by a factor of 2, assuming a symmetric distribution for the density of states, and possibly even further when E_F lies in an exponentially decreasing tail of an asymmetric $g(E)$. This means that our theoretical estimate of σ_2 for $K \approx 30\%$ could be reduced from $800 (\Omega \text{ m})^{-1}$ to perhaps 500 to 600

$(\Omega \text{ m})^{-1}$ which is quite comparable to our measured value of 300 to 400 $(\Omega \text{ m})^{-1}$. In contrast, available data on n -type Ge for a wide range of compensations and concentrations yield much smaller values of σ_3/σ_{\min} ranging between 10^{-2} and 10^{-3} for hopping processes.^{2,3,6}

The resistivity of the four remaining samples, which we have classified as metallic, is essentially independent of temperature except for the samples $M1$ and $M2$ shown in Fig. 2, which are closest to the transition. We note that in addition to giving information regarding the number of available carriers, the resistivity also reflects changes in their mobility. We suggest that the decrease in the resistivity observed for samples $M1$ and $M2$ as the temperature increases above about 50 K reflects predominantly an increase in the mobility associated with reduced scattering from ionized impurities. Further, the qualitative features of the high-temperature resistivity of the two samples straddling the transition, namely the insulating $I4$ sample and the metallic $M1$ sample, are very similar, and reflect the fact that at temperatures above approximately 50 K, electron transport for both takes place mainly in the conduction band.

Turning now to the Hall coefficients of the four insulating samples shown in Fig. 3, one notes that they exhibit different activation energies in the same two distinct ranges of temperature as the resistivity. These ranges are separated by a small maximum or inflection point in the Hall coefficient which signals a change from one dominant transport process to another. Except in the vicinity of these crossover regions (or at very low temperature), the Hall coefficient simply reflects the number of carriers, and not their mobility.

The activation energies ϵ_1^H and ϵ_2^H deduced from the Hall measurements for insulating samples $I1$ and $I2$ are listed in Table II. One should note that ϵ_1^H is generally smaller than the ϵ_1 deduced from the resistivity, since the latter reflects changes in mobility with temperature as well as changes in carrier number. The metallic samples, of which we have plotted only $M1$, exhibit no structure at all, indicating that the number of carriers is constant within the range of temperature and the accuracy of our measurements.

An interesting feature of our data for the insulating samples is that the Hall coefficient and the resistivity exhibit apparently different activation energies in the " ϵ_2 " range, namely, where the dominant mechanism is activation from the Fermi energy located in a D^0 impurity band of single occupancy states to a mobility edge in the D^- band of double occupancy states. Similar results have been observed in other materials. In particular, the

TABLE II. For samples $I1$ and $I2$, the parameters listed are ϵ_1 , ϵ_1^H , ϵ_2 , ϵ_2^H , and σ_2 . Here ϵ_1 , ϵ_2 , and σ_2 are determined by fitting the measured conductivity to $\sigma = \sigma_1 \exp(-\epsilon_1/kT) + \sigma_2 \exp(-\epsilon_2/kT)$. The values ϵ_1^H and ϵ_2^H are obtained from the measured Hall coefficient. Energies are determined to within 0.2 meV.

Sample	ϵ_1 (meV)	ϵ_1^H (meV)	ϵ_2 (meV)	ϵ_2^H (meV)	$\sigma_2 (\Omega \text{ m})^{-1}$
$I1$	8.7	5.4	2.7	2.2	290 ± 10
$I2$	6.2	4.3	2.3	1.3	380 ± 10

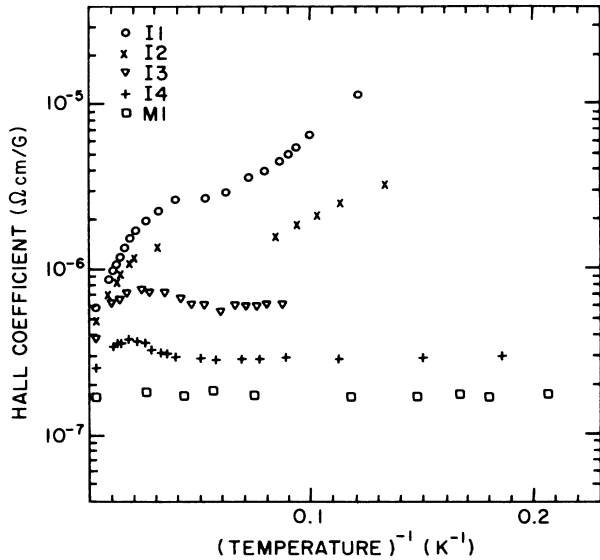


FIG. 3. Hall coefficient as a function of the inverse temperature for *n*-type CdSe samples *I1* to *I4* and *M1*.

activation energy deduced for sample *I2* from the Hall coefficient is about half as large as that deduced from the resistivity data. The same factor of approximately 2 was found by Fritzsche^{5,7} in his classic work on uncompensated (or low compensation) Ge:Ga over a reasonably extended range of dopant concentrations near the metal-insulator transition.

The magnetoresistance at 4.2 K of two insulating CdSe samples *I1* and *I4*, are plotted as a function of magnetic field up to 90 kG in Fig. 4. The resistivity decreases for fields up to about 50 kG and then increases at higher magnetic fields. Similar results were obtained for *n*-type CdSe by Jaroszynski and Dietl,⁸ who ascribed the nega-

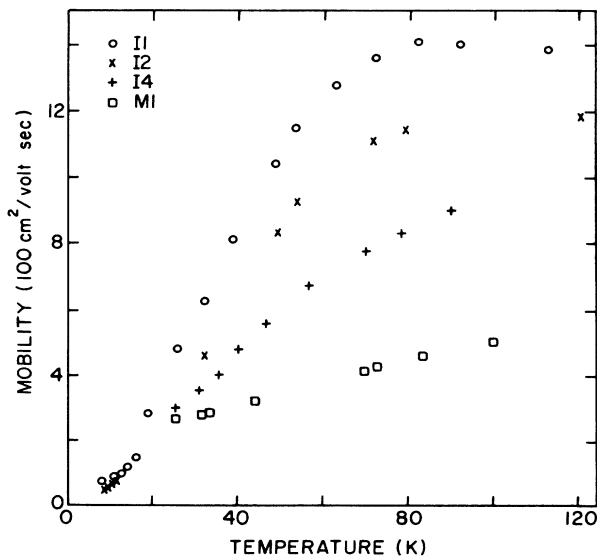


FIG. 4. Mobility vs temperature for three insulating (*I1*, *I2*, and *I4*) samples and one metallic *n*-type CdSe sample.

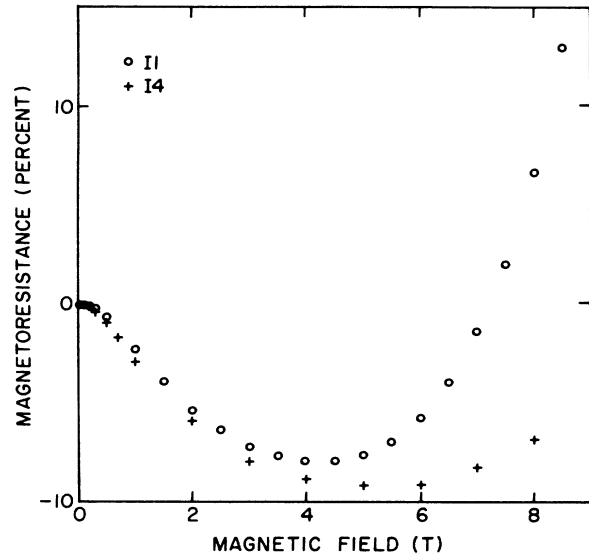


FIG. 5. The magnetoresistance at 4.2 K as a function of the magnetic field for two insulating *n*-type CdSe samples.

tive magnetoresistance at low fields to the delocalization associated with dephasing of backscattered waves, and the positive magnetoresistance to the shrinking of the donor wave functions and consequent shift in n_c at high magnetic fields.

B. Mobility and compensation

In this section we estimate the compensation for samples on both sides of the metal-insulator transition from the value of the Hall mobility in the conduction band. The various scattering mechanisms which determine the mobility will be discussed.

1. Insulating samples

Figure 4 shows a plot of the Hall mobility, calculated from the relation $\mu_H = R_H/\rho$, as a function of temperature for samples *I1*, *I2*, *I4*, and *M1*. For all samples, the mobility increases with increasing temperature between 15 and 90 K.

We have argued that both the Hall coefficient and the resistivity data indicate that at temperatures above about 50 K, transport occurs mainly in the conduction band for insulating samples *I1* to *I4*. As the temperature is lowered below 50 K, impurity band conduction begins to play an increasingly significant role.

In the temperature range between 50 and 100 K, ionized impurity scattering constitutes the dominant scattering mechanism determining the mobility of conduction electrons, although neutral impurity scattering also plays an important role. Piezoelectric scattering gives a small, but non-negligible contribution, which we take into account in determining compensation.^{9,10} Both polar-optical¹⁰ and acoustic-phonon¹¹ scattering are completely negligible below 80 K, although the first of these is comparable to piezoelectric scattering near 100 K.

The mobility due to ionized impurity scattering, μ_I , is

extracted from the Hall mobility μ_H , by using the relation

$$(1/\mu_I) = (1/\mu_H) - (1/\mu_N) - (1/\mu_{pz}), \quad (4)$$

where μ_N is the mobility due to neutral impurity scattering and μ_{pz} is the piezoelectric scattering mobility for CdSe. The mobility μ_N due to neutral impurity scattering is determined from Erginsoy's¹² formula:

$$\mu_N = \frac{e^3 m^*}{20 \hbar^3 \epsilon} \frac{1}{N_N}. \quad (5)$$

Here N_N is the density of neutral impurities, m^* is the conduction-band mass¹³ in CdSe, and ϵ is the dielectric constant.

The piezoelectric scattering mobility is given by Hutson,⁹

$$\mu_{pz} = \frac{16(2\pi)^{1/2}}{3} \frac{h^2}{em^*{}^{3/2}(k_B T)^{1/2}} \times \left[\sum_{\text{modes}} \left[\frac{(K^2)_{av}}{\epsilon} \right] \right]^{-1}, \quad (6)$$

where k_B is Boltzmann's constant, e is the electronic charge, and K is an electromechanical coupling constant. The summation refers to longitudinal and shear modes, and the averaging procedure is described in Ref. 9.

The assumption in Eq. (4) that the scattering processes which determine the mobility are independent of each other is not strictly valid. Corrections to this formula would give a higher value for μ_I and, consequently, a lower value for the compensation.^{14,15} We take the effect of electron-electron scattering into account in our determination of the compensation only for the metallic samples, where it plays a more significant role.

The compensation for the insulating samples *I1* and *I2* is obtained from the value of the mobility due to ionized impurity scattering by using the Brooks-Herring formula, suitably modified to take into account correlations between ionized scattering centers:¹⁶

$$\mu = 2^{7/2} \epsilon^2 (k_B T)^{3/2} [\pi^{3/2} m^*{}^{1/2} e^3 N_I f(x)]^{-1}, \quad (7)$$

where

$$f(x) = [\ln(1+x) - x/(1+x)]$$

and

$$x = 6m^* \epsilon (k_B T)^2 (\hbar^2 \pi n_s e^2)^{-1}.$$

Here ϵ is the dielectric constant, m^* is the effective conduction-band mass, N_I is the number of impurity centers ($N_I = n + 2N_A$), n is the number of carriers at temperature T , n_s is given by

$$n_s = n + (n + N_A)[1 - (n + N_A)/N_D], \quad (8)$$

and N_D and N_A are the number of donor and acceptor impurities, respectively. We have verified that we can indeed use the above formula, which is valid only for the nondegenerate limit, by comparing with results obtained from the expression of Mansfield¹⁷ for the case of arbitrary degeneracy.

A fit of our data for samples *I1* and *I2* to Eq. (7) allows us to obtain an estimate of the number of ionized impurity centers, $N_I = n + 2N_A$, from which we extract the number of acceptors N_A . The donor density can then be determined from the room-temperature Hall coefficient which gives the exhaustion-range electron density $n_0 = N_D - N_A$. This analysis yields estimates¹⁸ for the compensation $K = N_A/N_D$ of 0.2 to 0.25 for samples *I1*, and of about 0.35 for sample *I2*.

Comparisons with the predictions of the Brooks-Herring formula, and also of the modified theory of Falicov and Cuevas¹⁴ for low temperatures,^{19,20} with our experimental results for μ_I below 60 K indicate that as we lower the temperature the contribution of ionized impurity scattering to the mobility drops faster than predicted by the theoretical expressions. We believe that this is probably due to the increasing importance of impurity band conduction. Below 15 K, where transport takes place mostly in the D^- impurity band, the value of the mobility begins to saturate, as shown in Fig. 4, whereas the expression of Falicov and Cuevas predicts that μ_I goes to zero as $T \rightarrow 0$. Use of the Brooks-Herring formula at too low a temperature can, therefore, lead to erroneous determinations of the compensation ratio K .

2. Metallic samples

The compensation for metallic samples *M3* and *M4* is determined from the mobility in much the same way as in the case of *I1* and *I2*. However, we neglect neutral impurity scattering. This is justified to some extent by the fact that the Hall coefficient shows no freeze out of charge carriers.

The expression for μ_I is given in the degenerate limit by

$$\mu_I = \frac{3h^3 \epsilon^2 n_0}{16\pi^2 e^3 N_I m^*{}^2 f(x)}, \quad (9)$$

where all terms are defined above, but where x is now equal to $h^2 \epsilon (3n_0)^{1/3} / 2[e^2 m^* (8\pi)^{1/3}]$, and where we have lifted the condition that $n = N_I$ of Ref. 17.

Comparison with the results given by the full expression for arbitrary degeneracy confirms that these samples are indeed in the degenerate limit. Equation (9) is obtained by treating the electronic screening of the ionized impurities in the Thomas-Fermi approximation, and assuming no electron-electron scattering, nor any correlations between the impurity centers. Various treatments of electron scattering which improve upon the above result are discussed by Lax and Narayanamurti.²¹ All these schemes include the effects of electron exchange and correlations, but not of correlations between ionized impurity centers. These calculations are (1) the Green's-function technique of Toigo and Woodruff²² with a Hartree-Fock type of decoupling, (2) the Wigner distribution function method of Brosens, Lemmens, and DeVreese²³⁻²⁵ with a dynamic Hartree-Fock decoupling leading to a frequency dependent local-field correction $G(q, \omega)$; (3) an equation of motion technique of Singwi and co-workers²⁶⁻²⁸ with a decoupling based on a density-dependent equilibrium pair-correlation function

combined with a self-consistent calculation of the pair-correlation function $g(r)$ and $G(q)=G(q,\omega=0)$; (4) a perturbation (in the electron-electron coupling) analysis of exchange and correlation corrections by Holas, Aravind, and Singwi²⁹ which leads to a dynamical "local field" $G(q,\omega)$ that can be compared with Geldart and Taylor³⁰ and with Brosens, DeVreese, and Lemmens.²⁴

The corrections introduced by all these treatments can be neatly subsumed in the f function of the above expression for μ_I [Eq. (9)], so that the new expression for the ionized impurity scattering mobility becomes

$$\mu_I = \frac{3h^3\epsilon^2 n_0}{32\pi^2 e^3 N_I m^* f_{-1}(x)}, \quad (10)$$

where $f_{-1}(x)$ is a function different from the previous $f(x)$, and depends on the particular treatment of screening. For clarity, plots taken from Ref. 21 for $f_{-1}(x)$ are here reproduced in Fig. 6.

Table III shows the values of the compensation for samples *M3* and *M4*. We see that in all cases K is reduced from a Thomas-Fermi value of about 0.45 for both samples, to a value between 0.33 and 0.2, depending on the particular treatment. The calculation of Brosens *et al.* can give markedly different results from Toigo-Woodruff and Vashishta-Singwi, especially for small x .³¹

3. Discussion of uncertainties

Various authors have discussed the uncertainties^{14,16,17,32} involved in theoretical formulations for the ionized impurity scattering mobility in the nondegenerate case. Based on these works, we estimate the uncertainty in the compensations for insulating samples *I1*, and *I2* to be very approximately 20–30%.

Uncertainties in theoretical determinations of μ_I in the degenerate case have not been heretofore discussed in detail. There are three main sources of possible error: (1) errors incurred in extracting from the total measured mobility the mobility due only to ionized impurities; the largest contribution which we have neglected is due to piezoelectric scattering, which we estimate to be at most 5% of the total at the temperatures in question; (2) use of the Born approximation to calculate the scattering rate, where the criteria for its validity are only marginally satisfied on the metallic side; using as a guide estimates of uncertainties obtained in detailed studies of the nondegenerate case,³² we suggest that this could lead to errors on the order of 10, or at most 15%; and (3) different treatments of the screening, which yield values of compensation which differ by as much as 30% for samples *M3* and *M4*. Our overall estimate of the uncertainty is therefore very roughly 50%. It should be noted, however, that unlike the experimental error which is random

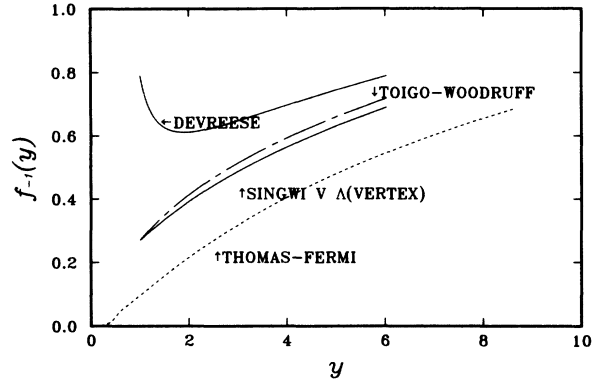


FIG. 6. Plot of function f_{-1} from Ref. 21. Labels indicate the particular screening treatment employed in the calculation.

and on the order of 5%, the uncertainty of 50% associated with the theoretical treatment is systematic in all instances. Thus, relative values of the compensation have been determined more reliably than their absolute values.

C. Comparison with other data for CdSe

Measurements of the resistivity and of the Hall coefficient as well as the magnetoresistance have been obtained by Finlayson *et al.*¹¹ for Cr-doped CdSe with electron concentrations comparable to ours. We note that the features of their Hall coefficient data differ from ours for carrier concentrations comparable to samples *I1* and *I2* of the present studies. Whereas in our data the ϵ_1 and ϵ_2 regions are separated by an inflection point and there is a non-negligible slope in the ϵ_2 region, their data exhibit a clear maximum separating both regions and fairly flat behavior in the range of impurity band conduction. Finlayson *et al.*¹¹ claim that their Hall coefficient data at these temperatures can be ascribed to conduction above the mobility edge in a single occupancy impurity band. The claim that only a single occupancy lower D^0 band exists is based on their conclusion that D^- levels are virtually nonexistent due to the very heavy compensation of their samples which they estimate, using the Brooks-Herring formula, at about 80%. We note, however, that we have applied this formula to their published values of the mobility at temperatures of 40 and 50 K, for their sample with $n_0 = 1.2 \times 10^{17} \text{ cm}^{-3}$, and we deduce compensations of 50% or less, which is considerably lower than the values they claim,³³ and which would imply that one may not be able to rule out the presence of a D^- band. Although we cannot definitely rule out the possibility that the D^- band is absent, we think it more likely that the observed differences originate with the different nature of the impurities ("magnetic" Cr compared to In)

TABLE III. Values of the compensation K for samples *M3* and *M4* deduced from different treatments of the electron screening, as discussed in detail in the text.

Sample	Thomas-Fermi	Vashishta-Singwi	Toigo-Woodruff	Brosens <i>et al.</i>
<i>M3</i>	0.45	0.32	0.29	0.22
<i>M4</i>	0.45	0.32	0.30	0.24

and/or the rather high densities of Cr added to the samples during the growth of their crystals.

IV. SUMMARY AND CONCLUSIONS

We have presented experimental data for the resistivity and Hall coefficient between about 8 and 80 K, and the magnetoresistance to 90 kG, of a series of CdSe samples with donor concentrations spanning the metal-insulator transition. The general features of the data, and measurements on selected samples to lower temperature (1.2 K) yield a critical carrier concentration for (compensated) CdSe of $(3.2 \pm 0.4) \times 10^{17} \text{ cm}^{-3}$, an energy ϵ_1 which we associate with carriers activated into the conduction band and an energy ϵ_2 which, we argue, is attributable to impurity band conduction at intermediate temperatures.

Using the Brooks-Herring formula for insulating material, and an appropriate expression for the ionized impurity scattering mobility in metallic samples we have used the measured Hall mobility to estimate the level of compensation of our In-doped CdSe material for metallic as well as insulating material.

To our knowledge, this is the first application of recent

theory to attempt to estimate compensation for metallic samples using transport data. Our data differ from earlier results on insulating Cr-doped CdSe of Finlayson *et al.* We argue that this difference is unlikely to be associated with the heavier levels of compensation claimed by the authors and is probably due to the different nature and very high density of the Cr present in their samples.

Note added in proof. Recent calculations by J. R. Meyer and F. J. Bartoli [Phys. Rev. B **36**, 5989 (1987)] for uncompensated materials indicate that multi-ion screening by electrons can lead to corrections to the theoretically predicted values of the electron mobility in degenerate semiconductors.

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$$\sigma_I = \frac{32\epsilon^2 m^* (k_B T)^3 f_2(\eta^*)}{N_I e^2 h^3 f(x)},$$

with

$$x = \frac{\bar{\eta}(kT)^{1/2} \epsilon h}{e^2 (2m^*)^{1/2} f'_{1/2}(\eta^*)},$$

where all the parameters are as defined in the text. Here

$$f_k(\eta^*) = \int_0^\infty \frac{x^k dx}{\exp(x - \eta^*) + 1}$$

(Fermi-Dirac functions), with

$$f'_k = \frac{d}{d\eta} f_k(\eta);$$

η^* is the reduced chemical potential $\eta^* = \mu/kT$, and $\bar{\eta}$ satisfies

$$(\bar{\eta} - 3) \exp(\bar{\eta} - \eta^*) = \bar{\eta} + 3.$$

It should be noted that Mansfield's expression does not take into account correlations between ionized scattering centers.

- ¹⁸Values for n_s and N_I (and thus, for $K = N_A/N_D$) were obtained from Eqs. (7) and (8) by starting with $n_s = n$ and iteratively adjusting N_I and n_s to be self-consistent.
¹⁹The results obtained from the Falicov and Cuevas expression [Eq. (2.17) of Ref. 16] for μ_I can only be considered as very approximate in our case since our samples do not meet their criterion that the density of ionized majority impurities approaches the same value as N_A . Nevertheless, we find that the compensation predicted by their formula is very close to the values given by the Brooks-Herring formula.
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