THE METAL — $Cd_xHg_{1-x}Te$ CONTACT. PART III. THE TRANSPORT MECHANISM*

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The values of parameters characterizing current flow through metal — $Cd_xHg_{1-x}Te$ contacts have been calculated and energy distribution of the current density determined. The prevailing transport mechanism of current carriers has been discussed. From the calculations performed, it follows that for contacts to (p) $Cd_xHg_{1-x}Te$ Thermionic Field Emission (TFE) and Thermionic Emission (TE) mechanisms prevailed at temperatures close to 77 K and 300 K, respectively. For contacts to (n) $Cd_xHg_{1-x}Te$ in the temperature range 77–400 K the TFE mechanism prevailed while at a temperature close to 77 K the Field Emission (FE) mechanism was predominant. It has also been emphasized that the results of experiments performed show a distinct influence of surface states on the properties of metal — $Cd_xHg_{1-x}Te$ contacts.

1. *Introduction*

Increasing interest in the properties of metal-semiconductor (M–S) contacts has taken place in the recent years as manifested by the numerous papers published yearly. The electric properties of contacts semiconductors of the n- and p-types as well as their photoelectric properties have been investigated (see e.g. [1–8, 31]). The basic mechanism of current flow through M–S contacts has been, among others, discussed in papers [9–11, 29]. Particular interest is now being show to rectifying junctions (the so-called Shottky's junctions). They can be used e.g. in field-effect transistors or as elements in high frequency electronic systems, since they do not have the defects of $p-n$ junctions (i.e. the defects related to limitations of the work speed due to the presence of minor carriers).

Results obtained from the investigations of some electric properties of the metal — $Cd_xHg_{1-x}Te$ contacts of p- and n-types have been described in our previous papers [12–14]. They have been used in the discussion of current transport mechanism in metal —

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$Cd_xHg_{1-x}Te$ contacts presented in this papers. The discussion was based on the results obtained for potential barrier transmission coefficients, and on the calculations of the energy distribution of electron density in current flowing through the contacts.

2. *Computational results and discussion*

2.1. Effective width of the potential barrier

Results of computations obtained for the width of the potential barrier on metal — $Cd_xHg_{1-x}Te$ contacts for different heights and concentrations of impurities are given in [13]. Since $Cd_xHg_{1-x}Te$ is a degenerated (for the x examined) semiconductor, the

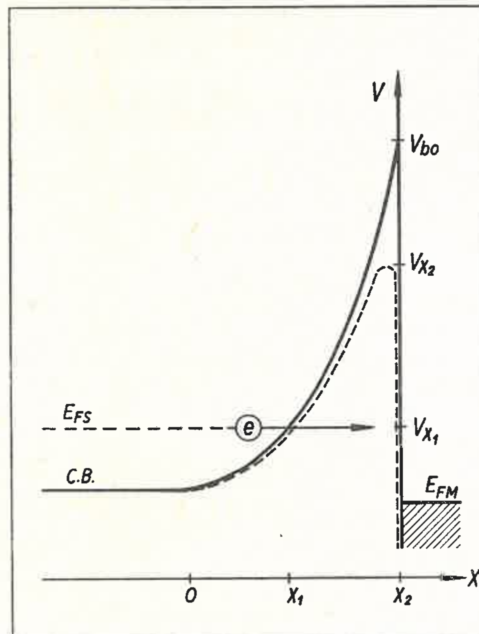

Fig. 1. Energy band diagram of metal-n type semiconductor used in computation

calculation of the effective barrier height, i.e. the width "seen" by the electron at the Fermi level, is very essential. The energy model of the contact under forward bias used in computation is presented schematically in Fig. 1. This model is a true representation of a contact barrier in a metal — n type semiconductor junction with $\varphi_s < \varphi_m$ but it can well illustrate the barrier on the contact with (p) $Cd_xHg_{1-x}Te$, when $\varphi_s > \varphi_m$ (the image is inverted). The distance $(x_2 - x_1)$ in Fig. 1 is just the effective width of the barrier for an electron on the Fermi level (on energy level qV_{x1}).

The barrier width has been calculated for the impurity concentration $N_D = 10^{23}$ m^{-3} and two temperatures 77 K and 300 K, using the well-known relations, (e.g. according to [5]):

$$t' = X_2 - X_1 = w\left[1 - \left(\frac{E_x}{qV_{bo}}\right)^{1/2}\right], \tag{1}$$

and

$$t = w\left[\left(1-\frac{\mathscr{V}_0}{1-E_x/qV_{b0}}\right)-\left(\frac{E_x}{qV_{b0}}+\frac{\mathscr{V}_0}{1-E_x/qV_{b0}}\right)^{1/2}\right], \tag{2}$$

where $w = \left(\frac{2\varepsilon_s V_{b0}}{qN}\right)^{1/2}$ is a well-known formula for the width of a parabolic barrier with height V_{b0}, $V_b = V_{x2}$, and [11]

$$\mathscr{V}_0 = \frac{1}{16\pi}\left(\frac{N}{2}\right)^{1/2}\left(\frac{q}{\varepsilon_s V_{b0}}\right)^{3/2}. \tag{3}$$

The values t' (effective width of the parabolic barrier) and t (effective width for a barrier modified by imaging forces) are shown in Fig. 2. It should be noted that the barrier width is

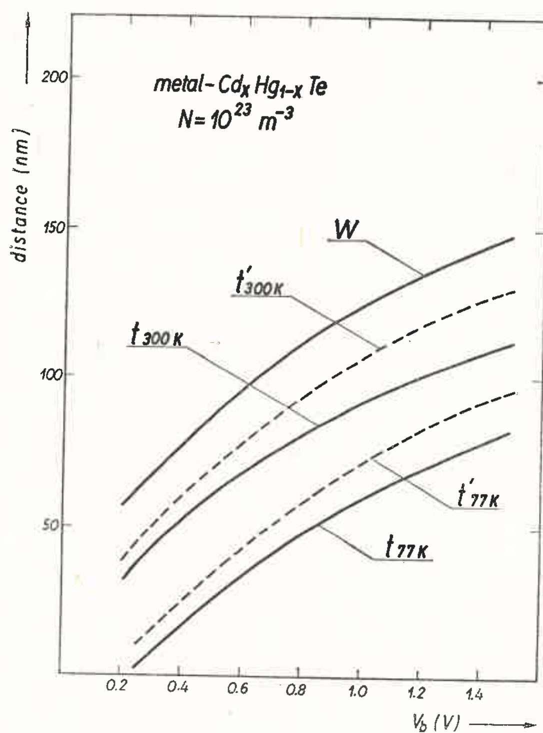

Fig. 2. Width of the potential barrier (notation — see the text)

relatively small, in particular for low height and at 77 K. The effective width of the barrier is considerably smaller than the width of the depletion region, denoted by w in Fig. 2, e.g. for $N_D = 10^{23}$ m^{-3} and $V_b = 0.5$ V we have obtained $t/w = 0.30$ and 0.45 at 77 K and 300 K, respectively.

2.2. The value of E_{00}

The quantity E_{00}/kT is very useful for a preliminary estimate of the mechanism predominant in current flow through the M–S contact [10, 15, 29]. Within the temperature interval in which tunnelling electrons have an energy lower than the barrier width in the contact (for the parabolic relation $E(\vec{k})$) the I–V characteristic under forward bias has the shape [15]

$$J = J_s \exp(qV/E_0), \tag{4}$$

where

$$E_0 = E_{00} \coth(E_{00}/\mathrm{kT}),$$

and

$$E_{00} = \tfrac{1}{2} q\hbar \left(\frac{N}{\varepsilon_s m^*}\right)^{1/2}. \tag{5}$$

In (5) N denotes the concentration of impurities, ε_s — dielectric constant of the semiconductor and m^* – effective mass of the carriers.

For low voltages, considerably lower than the barrier height $qV_b(V \ll V_b)$, the quantity E_{00} must be replaced by the quantity $\overline{E}_{00}$, which (using a two-band model) will be given by formula [16]:

$$\overline{E}_{00} = E_{00}\left(1 - q\,\frac{V_b - V - \xi}{E_g}\right)^{1/2}, \tag{6}$$

where $\xi = E_{FS}/q$, (E_{FS} is a Fermi level in semiconductor). Then

$$\overline{E}_0 = \overline{E}_{00} \coth\left(\frac{\overline{E}_{00}}{kT}\right). \tag{7}$$

The quantity E_{00}/kT (or $\overline{E}_{00}/kT$) can be now used to approximately determine which kind of transport mechanism predominates in the contact. If (TE) mechanism prevails,

TABLE I

The values of E_{00} and q/E_0 for metal — $Cd_xHg_{1-x}Te$ contacts

Doping concentration (m^{-3})		E_{00} in (eV)		q/E_0 in (V^{-1})	
		77 K	300 K	77 K	300 K
n-type	$N_D = 10^{22}$	0.00472	0.00403	129	38
	$N_D = 5\times10^{22}$	0.00905	0.00825	77	37.5
	$N_D = 10^{23}$	0.0117	0.0107	53	36.5
p-type	$N_A = 5\times10^{22}$	0.00132	0.00132	149	40
	$N_A = 10^{23}$	0.00186	0.00186	147	38.5
	$N_A = 10^{24}$	0.00590	0.00590	121	37.8

then $E_{00}/kT \ll 1$; for the prevailing (FE) mechanism $E_{00}/kT \gg 1$; if however (TFE) mechanism dominates, then $E_{00}/kT \cong 1$.

To estimate the value of E_{00} from formula (5) for the (*n*) $Cd_xHg_{1-x}Te$ (for $x \cong 0.2$), it has been assumed that $E_g = 0.16$ eV [17], $\varepsilon_s = 18\varepsilon_0$ (static dielectric constant according

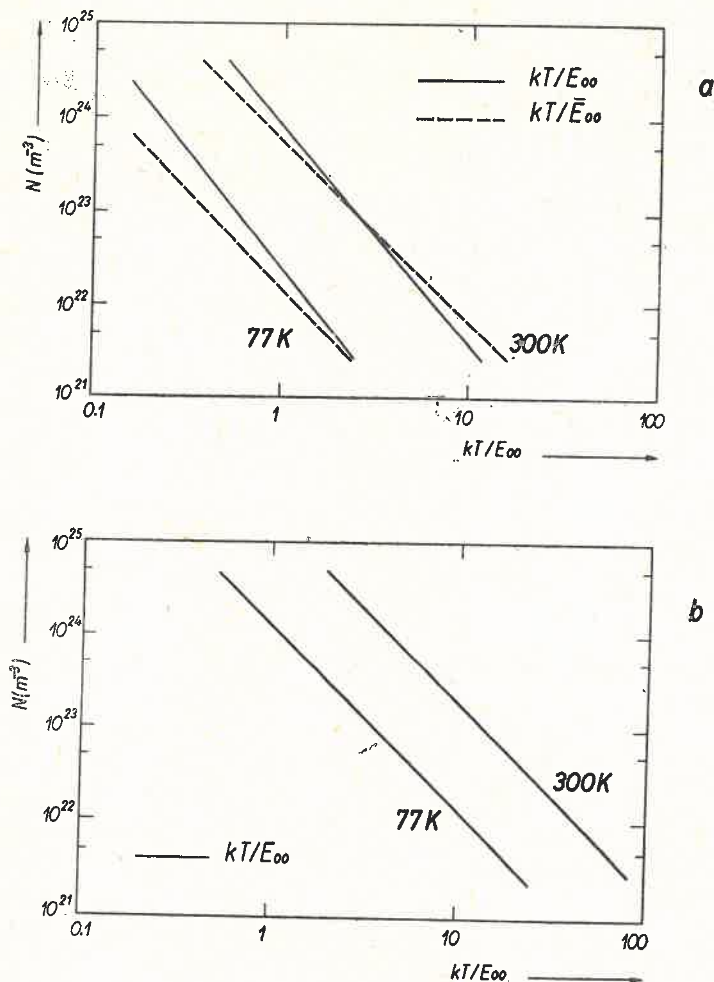

Fig. 3. The dependences of kT/E_{00} (and $kT/\bar{E}_{00}$) vs doping concentration for: a — (*n*) $Cd_xHg_{1-x}Te$ and b — (*p*) $Cd_xHg_{1-x}Te$

to [18]), m_e^* (at 77 K) = $0.012\, m_0$ and m_e^* (at 300 K) = $0.016\, m_0$ [19]. The respective values of E_{FS} for different temperatures and concentrations have been assumed according to [20]. For (*p*) $Cd_xHg_{1-x}Te$ the calculations have been performed by assuming $m_h^* = 0.55\, m_0$ [30] and $E_{FS} = -E_g$.

The values of E_{00} and q/E_0 computed for the temperatures 77 K and 300 K are presented in Table I. The kT/E_{00} values as a function of impurity concentration in (*n*) and (*p*)

$Cd_xHg_{1-x}Te$ at 77 K and 300 K are shown in Fig. 3. It should be noted that the slope of the current-voltage characteristic (i.e. the q/E_0 value) at 300 K depends weakly on the concentration of impurities for both types of conductivity.

2.3. The transmission coefficient of potential barrier

Density of the current flowing through the metal-semiconductor contact can be expressed [21] by the equation

$$J = \int_0^\infty J(E_x)dE_x = \int_0^{qV_b} J_1(E_x)dE_x + \int_{qV_b}^\infty J_2(E_x')dE_x, \tag{8}$$

where E_x is a component of kinetic energy of the electron, normal to the surface of the M–S contact, qV_b is the barrier height calculated from the Fermi level under equilibrium conditions, $J_1(E_x)$ and $J_2(E_x')$ denote the resultant current densities introduced by electrons in the energy range between E_x and (E_x+dE_x), and E_x' and $(E_x'+dE_x')$, respectively, (with $E_x < qV_b$ and $E_x' > qV_b$), given by the formulae

$$J_1(E_x)dE_x = P_1(E_x, m^*)N(E_x)dE_x, \quad J_2(E_x')dE_x = P_2(E_x', m^*)N(E_x')dE_x, \tag{9}$$

where $N(E_x)dE_x$ and $N(E_x')dE_x$ represent resultant densities of the flux of electrons, normal to the contact. $P_1(E_x, m^*)$ is the barrier transmission coefficient for tunnelling electrons, given by the following formula (acc. to [22])

$$P_1(E_x, m^*) = \left\{1+\exp\left(\frac{8m^*}{2}\right)^{1/2} \int_0^t [qV_b(x)-E_x]^{1/2}dx\right\}^{-1}, \tag{10}$$

where t is the length of the tunnelling path for the energy level E_x. $P_2(E_x', m^*)$ is the transmission coefficient for electrons passing over the barrier, given by (see cf. [5])

$$P_2(E_x', m^*) = 1-P_1(E_x, m^*), \tag{11}$$

where $E_x' = 2qV_b-E_x$.

For the electrons flowing from the semiconductor to the metal (forward bias) the value $N(E_x)$ is given by (acc. to [21])

$$N(E_x) = \frac{A_s^*T}{k}\left\{\ln\left[1+\exp\left(\frac{E_{FS}-E_x}{kT}\right)\right] - \ln\left[1+\exp\left(\frac{E_{FS}-E_x-qV}{kT}\right)\right]\right\}, \tag{12}$$

and for electrons flowing from the metal to the semiconductor by, (acc. to [5])

$$N(E_x) = \frac{A_M^*T}{k}\left\{\ln\left[1+\exp\left(\frac{E_{FM}-E_x}{kT}\right)\right] - \ln\left[1+\exp\left(\frac{E_{FM}-E_x-qV}{kT}\right)\right]\right\}, \tag{13}$$

for $E_x > E_{FM}$. A_s^* and A_M^* in (12) and (13) denote the effective Richardson constants for the semiconductor and metal, respectively. The transmission coefficient $P_1(E_x, m^*)$ has been calculated by applying the approximated formula, (acc. to [5])

$$P_1 \cong (1+\exp Q)^{-1}, \tag{14}$$

where

$$Q = Q(\mathscr{V}) = \frac{8\pi V_b}{h}\left(\frac{m^*\varepsilon_s}{N}\right)^{1/2}\left[(\mathscr{V}_m-\mathscr{V})^{1/2}\left(1-\frac{\mathscr{V}_0}{1-\mathscr{V}}-\frac{\mathscr{V}_m^{1/2}}{2}\right)\right.$$

$$\left.-\frac{\mathscr{V}}{2}\ln\frac{\mathscr{V}_m^{1/2}+(\mathscr{V}_m-\mathscr{V})^{1/2}}{\mathscr{V}^{1/2}}\right]. \tag{15}$$

The value of $\mathscr{V}_0$ in (15) can be obtained through formula (3), $\mathscr{V} = E_x/\mathscr{V}_b$ and $\mathscr{V}_m = V_{x2}/\mathscr{V}_{b0}$.

The calculations of the transmission coefficient P_1 have been performed for the parameters of $Cd_xHg_{1-x}Te$ given in Table II. The results are shown in Fig. 4. The values of P_1 are given as a function of the reduced energy $\mathscr{V}$ of the tunnelling electrons. The

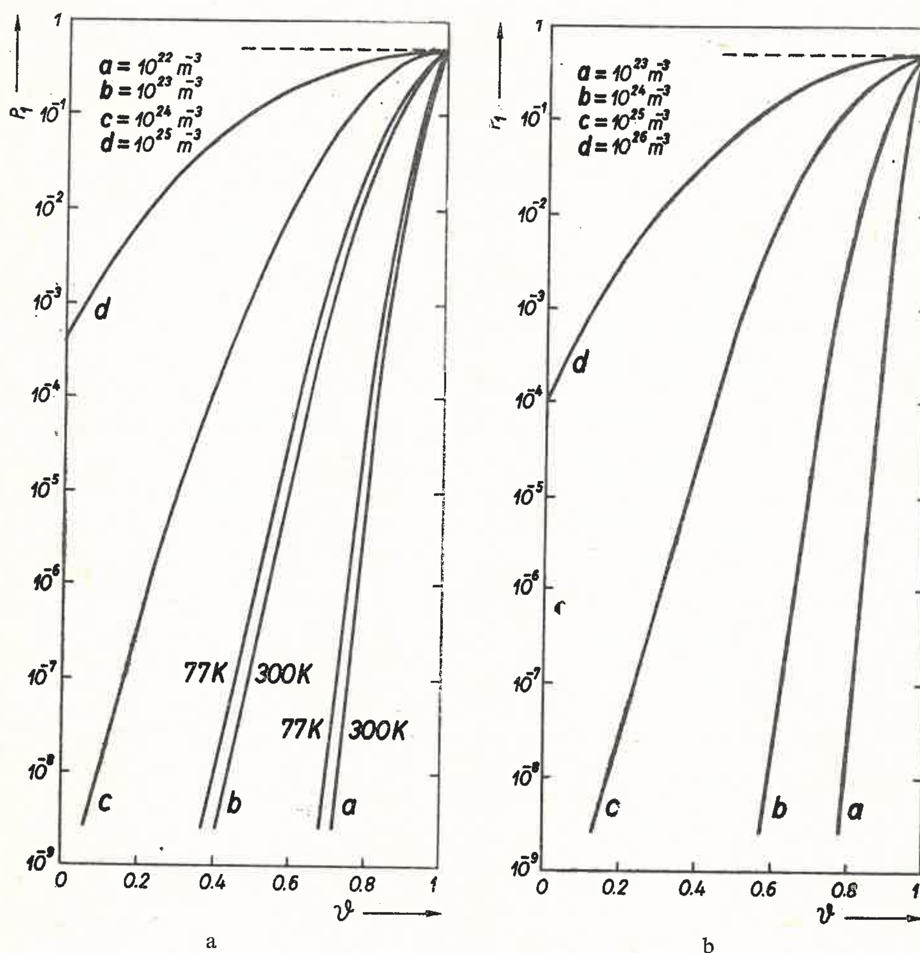

Fig. 4. The transmission coefficient P_1 vs reduced energy of an electron $\mathscr{V} = E_x/V_b$ for: a — (*n*) $Cd_xHg_{1-x}Te$ and b — (*p*) $Cd_xHg_{1-x}Te$

TABLE II

Data employed in computation

Doping concentration in (m^{-3})		Fermi level in (eV) 77 K	Fermi level in (eV) 300 K	Values of $(m^*/N)^{1/2}$ in ($kg^{1/2}\ m^{3/2}$) 77 K	Values of $(m^*/N)^{1/2}$ in ($kg^{1/2}\ m^{3/2}$) 300 K
n-type	$N_D = 10^{22}$	0.065	-0.050	1.0×10^{-27}	1.17×10^{-27}
	$N_D = 10^{23}$	0.170	$\cong 0$	4.05×10^{-28}	4.37×10^{-28}
	$N_D = 10^{24}$	$\cong 0.45$	0.13	1.84×10^{-28}	1.84×10^{-28}
p-type	$N_A = 10^{23}$			2.24×10^{-27}	2.24×10^{-27}
	$N_A = 10^{24}$	-0.10[a]	-0.16[a]	7.075×10^{-28}	7.075×10^{-28}
	$N_A = 10^{25}$			2.24×10^{-28}	2.24×10^{-28}

[a] Exact data are presently unknown.

values of the coefficient P_2 have been calculated by applying Kemble's approximation, i.e. from formula (11). The values of P_1 (and P_2) are practically independent of temperature for contacts to (p) $Cd_xHg_{1-x}Te$ within the whole range, because of the assumed constancy of the effective mass of the holes. The figures presented allow an easy estimation of the degree of transparency of the investigated barriers.

2.4. Energy distribution of electrons

Calculation of the P_1, P_2 and $N(E_x)$ values allowed one to calculate the energy distribution of electrons flowing through the metal — $Cd_xHg_{1-x}Te$ contact. Before the calculations were performed the appropriate values of the barrier heights on contacts had to be assumed. This requires knowledge of the value of the work function for $Cd_xHg_{1-x}Te$.

The values of work function for various compositions of $Cd_xHg_{1-x}Te$ are not yet known. The value of φ_s obtained from the measurements performed for heavily doped p-type CdTe (for $x = 1$) amounted to 6.0 eV [23]. This is in good agreement with the value of electron affinity $\mathscr{H} = 4.5$ eV, found for CdTe in [24]. For thin CdTe films with the concentration approaching the intrinsic one, the value found for φ_s amounted to 5.1 ± 0.1 eV [25]. For $Cd_{0.2}Hg_{0.8}Te$ in [13] the assumed value of $\varphi_s = 4.2$ eV. From the analysis of the above data it might be inferred that the values of work functions of the metal (φ_m) and of $Cd_xHg_{1-x}Te$ used in investigations (φ_s) satisfied fairly well the inequality $\varphi_s \geqslant \varphi_m$, except for Pt($\varphi_m = 5.3$ eV). With such a relation of the work functions for the n-type semiconductor the lack of a potential barrier or even the enriched layer formed at the contact [26] can be expected.

While analyzing the barrier height between the contacts, the effect of surface states should also be taken into consideration. For n-type $Cd_{0.2}Hg_{0.8}Te$ with the concentration $N_D = 7\times10^{20}\ m^{-3}$ (at 77 K) the density of surface states D_{ss} determined in [27] amounted to $2.1\times10^{16}\ eV^{-1}\ m^{-2}$. In paper [14] the density of surface states for the metal — (p)$Cd_xHg_{1-x}Te$ contacts, with concentrations $p = 10^{23}-10^{24}\ m^{-3}$ (at 77 K), was estimated

as $D_{ss} = (3.4 \pm 1.2) \times 10^{17}\ m^{-2}\ eV^{-1}$. This value is comparable with the values obtained for other contacts: (1.6 ± 1.1 for M–CdS, 2.7 ± 0.4 for M–GaP, 2.7 ± 0.7 for M–Si and 12.5 ± 10 for M–GaAs) quoted in [28] (all the values $\times 10^{17}\ m^{-2}\ eV^{-1}$).

In view of the identical, in practice, technology used by us for M–$(n)Cd_xHg_{1-x}Te$ and M–$(p)Cd_xHg_{1-x}Te$ junctions we assume that the density of surface states in contacts to $(n)Cd_xHg_{1-x}Te$ amounted also to $3 \times 10^{17}\ m^{-2}\ eV^{-1}$, approximately. The value of band curving at the $Cd_xHg_{1-x}Te$ surface caused by the charge of state surfaces amounted to $\psi_0 = 0.07$ eV [27]. Considering a similar ratio of surface states impurity concentrations in the semiconductor volume D_{ss}/N_D, and on the grounds of [27] it may be supposed that the value of band curving, caused by the presence of surface states in the $(n)\ Cd_xHg_{1-x}Te$ examined satisfies the inequality $\psi_0 < 0.1$ eV. Thus, in view of the relation $\varphi_s \geqslant \varphi_m$ and the conjectural value ψ_0 it seems that the potential barrier (resulting from the difference between work functions) did not appear on the M–$(n)Cd_xHg_{1-x}Te$ contacts, but it is quite probable that there appeared a barrier caused by surface states of $Cd_xHg_{1-x}Te$ whose height probably did not exceed 0.1 eV. This suggestion is partially confirmed by the results obtained from the measurements of I—V characteristic and of the capacitance of the M–$(p)Cd_xHg_{1-x}Te$ contacts [13]. The I—V characteristics were linear, while the capacitance values for e.g. $N_D = 10^{22}\ m^{-3}$ ranged within 45—75 pF, i.e. about one order of magnitude smaller than the values estimated from the contact geometry and parameters of material, assuming the existence of a depletion region i.e. for $\varphi_s < \varphi_m$. It has also been

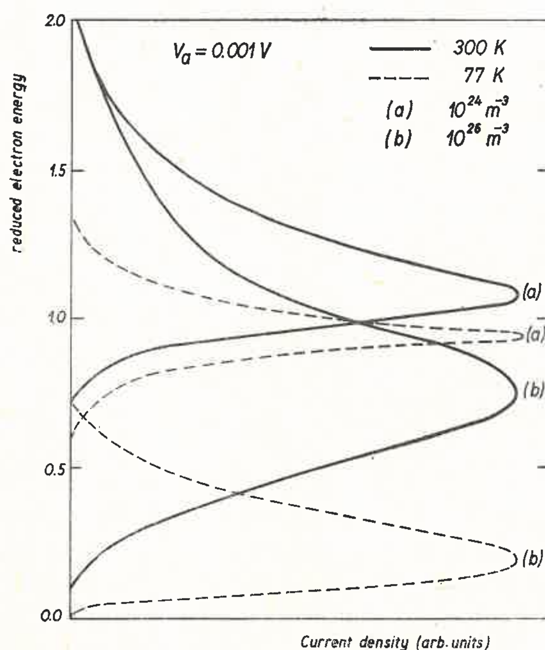

Fig. 5. Energy distribution of the hormalized current flowing through the metal — $(p)\ Cd_xHg_{1-x}Te$ contact under forward bias

added, that (on the other hand) the accumulation layer can exist on a surface of $Cd_xHg_{1-x}Te$ with small x [34] can lead to decay of the potential barrier on the metal — $Cd_xHg_{1-x}Te$ contact. For the $M-(p)Cd_xHg_{1-x}Te$ contacts, maximal barrier height has been stated for In, $qV_b \cong 0.55$ eV [14].

To calculate the current distribution, the values 0.1 eV and 0.55 eV have been assumed as the barrier heights on $M-(n)S$ and $M-(p)S$ contacts, respectively. Energy distributions of current density have been calculated according to formulae (8), (9), (12) and (13) for forward and reverse bias, for a few values of impurity concentrations and the voltages: 0.001 V, 0.01 V, 0.075 V, 0.150 V and 0.30 V for $M-(p)Cd_xHg_{1-x}Te$ contacts, and 0.001 V, 0.01 V and 0.05 V for $M-(n)Cd_xHg_{1-x}Te$ contacts, at 77 K and 300 K. Detailed results of the calculations obtained for the above parameters have been presented in [32]. Exemplary results obtained for the metal — $(p)Cd_xHg_{1-x}Te$ contacts under forward bias are presented in Fig. 5.

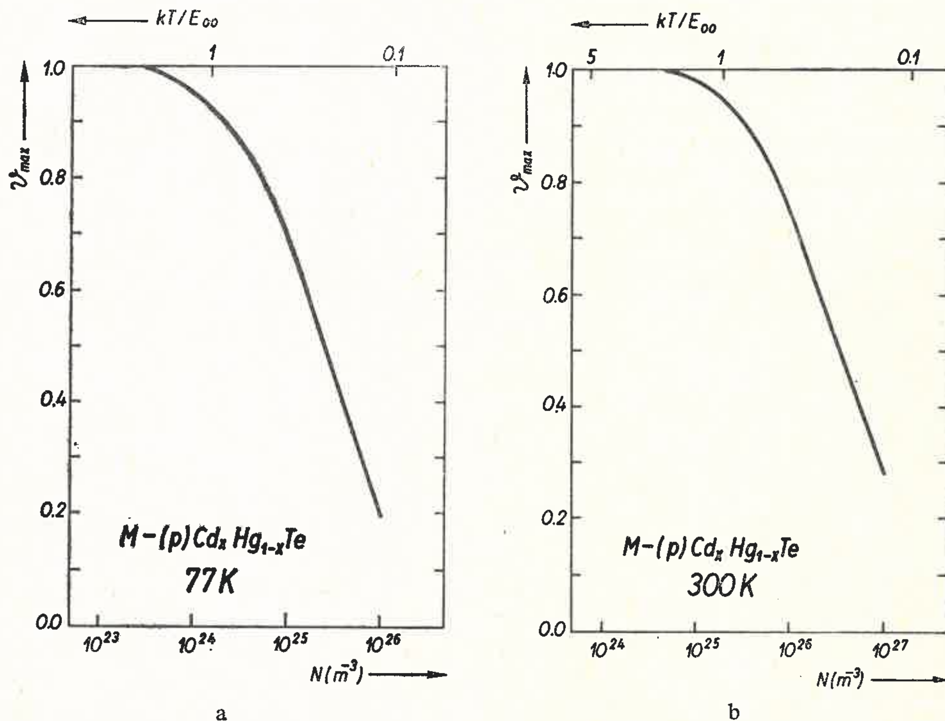

Fig. 6. Relative position of the current distribution maximum vs various doping concentration in (p) $Cd_xHg_{1-x}Te$

The results of current-energy distribution obtained from the calculations have shown the participation of thermionic and field emission mechanisms, respectively. In the case when tunnelling was the prevailing mechanism the electron distribution was strongly influenced by impurity concentration, temperature and voltage applied. This distribution is peaked at the maximum of relative electron energy $\mathcal{V}_{max}$ as shown in Fig. 5. For

comparative reasons, $\mathscr{V}_{max}$ plotted versus doping concentration for metal — $(p)Cd_xHg_{1-x}Te$ contacts is shown in Fig. 6. From this curve the participation of dominant current transport mechanism can be estimated. This estimation is consistent qualitatively with the computation of kT/E_{00} value vs doping concentration and dominant transport mechanism, obtained from this relation.

3. *Final conclusions*

The calculations of electron energy distribution in current flowing through the contact allow one to determine the dominant current transport mechanism in the contacts examined

a. metal – $(p)Cd_xHg_{1-x}Te$, the assumed barrier height 0.55 eV

At 77 K and for low concentrations the TE mechanism prevails; for $N \geqslant 10^{23}$ m^{-3} the participation of tunnelling becomes considerable and there occurs a TFE mechanism. With increasing temperature the dominance of TE mechanism is also growing (for the same concentrations). Visible participation of tunnelling at 300 K is observed when the concentration is near 10^{25} m^{-3}.

b. metal – $(n)\ Cd_xHg_{1-x}Te$, the assumed barrier height is 0.1 eV

At 77 K and for relatively low concentrations ($10^{21}-10^{23}$ m^{-2}) the TFE mechanism occurs with the contribution of tunnelling, the latter increases with increasing concentration. For $N \geqslant 10^{24}$ m^{-3} the contribution of thermionic emission current becomes negligibly small, (FE mechanism). The increased temperature is accompanied by an increased contribution of thermionic emission. Within the concentration range $10^{22}-10^{25}$ m^{-3} the TFE mechanism at 300 K is observed; for $N = 10^{21}$ m^{-3} the contribution from tunnelling is negligible.

A noticeable effect of surface states of $Cd_xHg_{1-x}Te$ on electrical properties of the contacts examined can be inferred from a few facts. The first is the dependence of the potential barrier height qV_{b0} on the work function of the metal φ_m, determined experimentally, $qV_{b0} = -0.2\ \varphi_m + 1.25$ (eV) [14]. Although the coefficient of the slope determined from the relation $qV_{b0}(\varphi_m)$ was not very accurate, it nevertheless was considerably smaller than unity which is characteristic of the simple Schotty's model, without the participation of surface states.

The second fact is the difference between the calculated values of slope coefficient of I—V characteristic (cf. Eq. (4) and Table I), and the values determined experimentally which were 2—3 times smaller [14]. This may be associated with the effect of recombination and trapping of surface states or traping centers in a semiconductor within the near-contact depletion region.

It has been also stated that $qV_{c0} > qV_{b0}$ (qV_{c0} is the barrier height obtained by a linear extrapolation C^{-2} vs V plot; qV_{b0} is the barrier height obtained from I—V characteristic) [14]. This fact also confirms, though indirectly, the existence of the interface states.

A high value of n factor, $n > 1$, (n is a factor on the equation of I—V characteristic, see, e.g. [14]) can also indicate a relatively strong effect exerted by surface states on electrical properties of the contacts examined. On the other hand, the n-value exceeds unity because of the effects of image forces and edge current leakage; even larger deviations of n from

unity arise due to tunneling of carriers through the contact [10, 11, 33]. At present the effect of surface states on electrical properties of metal — $Cd_xHg_{1-x}Te$ contacts cannot be explained sufficiently and additional research is required.

Additional factors which have a basic meaning for electrical properties of metal — $Cd_xHg_{1-x}Te$ contacts (especially, with small x) are a generation — recombination mechanism in the near-contact region.

It has been shown [35] that in n-type $Cd_xHg_{1-x}Te$ ($0.195 < x < 0.210$), for pure material ($N_D - N_A \gtrsim 4\times10^{20}$ m^{-3}, $\mu_H \gtrsim 15$ m^2 V^{-1}s^{-1} at 77 K) the carrier lifetime in the intrinsic conditions is determined by an Auger limited band-to-band process. In more compensated material ($N_D - N_A < 4\times10^{20}$ m^{-3}, $\mu_H < 15$ m^2 V^{-1}s^{-1} at 77 K) Shockley--Read limited process is observed.

The process, mentioned above, can carry in their contribution to measured electrical characteristics, due to additional generation – recombination current.

Some influence on these characteristics will also be exerted by trapping effects which have been stated in $Cd_xHg_{1-x}Te$ with small x in paper [36] as well as by impact ionization in high electric fields near the contact region. This latter effect has already been observed in narrow-gap semiconductors (e.g. in InSb [37] and in n-type $Cd_xHg_{1-x}Te$ [36] for electric fields above 1.6×10^3 Vm^{-1}).

All the above mentioned factors must be taken into consideration in the analysis of experimental results for the contacts examined. However, no use could be made of them in the calculation presented in this paper due to the simplicity of the model used.

The results obtained from calculation are therefore (in the above sense) approximate only, nevertheless they may help to understand the transport mechanism in metal — $Cd_xHg_{1-x}Te$ contacts.

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