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Temperature dependence of the R_0A product for photovoltaic PbTe detectors

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In the paper the limiting values of the R_0A product have been calculated for diffusion *p-n* PbTe junctions within the temperature range 77-300 K. The influence of the diffusion current (for the radiative and Auger recombination) and the generation-recombination current upon R_0A is discussed. The calculations have been carried out for optimum doping concentrations, for which the contribution of tunnel current component may be neglected. Also the calculations of R_0A for the Schottky junction are performed. The results of calculations are compared with the experimental data reported by other authors. A satisfactory consistence has been achieved for *p-n* junctions. An attempt was made to explain the divergences which appear for Schottky junctions. The working conditions for photovoltaic detectors, the detectivity of which is limited by the background radiation, were determined.

Introduction

The semiconductor lead chalcogenide compounds find a wide application in optoelectronics as detectors and sources (lasers) of infrared radiation. Due to the difficulties in the production of materials of low concentration and the short lifetime of the carriers in those compounds the main effort is directed toward the production of the photovoltaic detectors.

PbTe is a semiconductor on the base of which the photovoltaic detectors (*p-n* junction [1-8], and Schottky junctions [9-12]) are produced for the spectral range 3-5 μm. In the paper [13] the influence of the doping concentration on the R_0A product (differential resistance — zero-volt bias — times the junction area) has been analysed for the abrupt *p-n* PbTe junctions.

In the present paper the limiting values of R_0A for the abrupt p-n PbTe junction were determined for the temperature range 77-300 K. The calculations were carried out for the optimum doping concentration for which the carrier tunnelling may be neclected. The influence of the diffusion and generation-recombination current in the depletion layer upon the R_0A product has been considered. A comparison of the abrupt *p-n* junction with that of Schottky type is made. The results of considerations are confronted with the experimental data reported by other authors.

Abrupt *p-n* junction

The total density of dark current flowing through the junction may be written in the form

$$J = J_D + J_{GR} + J_T + J_Z, \tag{1}$$

where the particular components denote respectively: diffusion current density, generation-recombination current density in the depletion layer, tunelling current density and leakage current density. For the optimum doping concentrations, considered in this paper, the contribution of the tunnelling component may be neglected. The Z component may be caused by both volume and surfaces defects of the material. For a suitable technology and design of the diode the influence of the J_Z component is unessential.

The R_0A product determined by the diffusion current in the case of radiative recombination is [14]:

$$(R_0A)_R = \frac{(kT)^{1/2}}{q^{3/2} n_i^2 \mu^{1/2} R^{1/2}} \sqrt{n_{\mathrm{ef}}}, \tag{2}$$

where n_{ef} — $np/(n+2\sqrt{np}+p)$ — effective doping concentration,
μ — average values of the mobility of electrons and holes,
n_i — intrinsic concentration,
q — electron charge,
R — coefficient of radiative recombination.

The intrinsic concentration is determined by the formula [15]:

$$n_i = 2[2\pi kT/h^2]^{3/2} [m_{dn}^* m_{dp}^*]^{3/4} \exp[-E_g/2kT], \tag{3}$$

where m_{dp}^* and m_{dn}^* denote the density-of-states effective masses, and E_g — energy gap. The formula (3) is valid for $E_g \gg kT$, being fulfilled in the case of PbTe. The values of density-of-effective masses state may be determined when knowing the longitudinal and transversal components of the effective mass, since $m_d^* = N^{2/3}[m_l^* m_t^{*2}]^{1/3}$. For the lead chalcogenides the number of equivalent extremes in the conduction and valence bands is equal to 4.

Due to the mirror symmetry of the conduction and valence bands the values of effective masses of the electrons and holes are close to each other $m_e^* \simeq m_h^*$. In this case the coefficient of radiative recombination $R = R_n = R_p$, and, as it is shown in [16], amounts to

$$R = \frac{1\times 10^{-15}\bar{n}E_g^2}{[kT]^{3/2}K^{1/2}[2+1/K]^{3/2}[m^*/m_0]^{5/2}}, \tag{4}$$

where $\bar{n}$ denotes the refractive index, $K = m_l^*/m_t^*$ is the coefficient of anisotropy of effective masses, m_0 is the mass of free electron. The mass m^* may be determined from the formula $m^* = [1/3(2/m_t^* + 1/m_l^*)]^{-1}$. In the formula (4) kT and E_g are expressed in electronovolts. For the Auger recombination [14]:

$$(R_0A)_A = \frac{(kT)^{1/2}}{2q^{3/2} n_i^2 \mu^{1/2} C^{1/2}}. \tag{5}$$

The Auger recombination coefficient $C = C_n = C_p$ has the form [17]:

$$C = \frac{1}{(2\pi)^{1/2}} \frac{N'}{N^2} \frac{q^4}{\varepsilon_\infty^2} [kT]^{1/2} E_9^{-7/2} \frac{h^3}{m_l^{*1/2} m_t^{*3/2}} \exp\left[-\frac{E_g K^{-1}}{2kT}\right], \tag{6}$$

where ε_∞ is a high-frequency dielectric constant, and $N' = 3$ is the number of valleys, to which the energy scatter from a given valley may occur.

The R_0A product, denoted by the generation-recombination region of the depletion layer in the abrupt junction, is [18]:

$$(R_0A)_{GR} = \frac{E_g^{1/2}\tau_0}{qn_i(2\varepsilon_s)^{1/2}} \sqrt{n'_{\mathrm{ef}}}, \tag{7}$$

where ε_s denotes the static dielectric constant and $n'_{\mathrm{ef}} = np/(n+p)$ is the effective concentration.

In the formula (7) τ_0 (the time determining the recomination by the Shockley-Read centers) is a parameter difficult to determine. The Shockley-Read centers cannot be of hydrogen-like nature because great dielectric constant would cause their shift toward the band edge and then their influence on the lifetime would be quite small. It can be only suggested that these centres are positioned within the energy gap and are not connected with the electrically active defects [18].

Schottky's junction

The product R_0A for the Schottky's junction is determined by [19]:

$$(R_0A)_{M\text{-}S} = \frac{kT^{-1}}{qA^*} \exp\left[\frac{\varphi_B}{kT}\right], \tag{8}$$

where φ_B denotes the barrier height and A^* is the Richardson constant.

The formula (8) is valid for an ideal M-S junction under the following assumptions: i) the barrier height is much greater than kT, and ii) the collisions in the barrier region and such phenomena as the influence of the image forces, tunnelling through the upper part of the barrier and penetration of the barrier by the surface states, are neglected.

In the papers [20] and [12] it has been pointed out that in the case of a metal-semiconductor junction with narrow energy gap and for the hole-type conduction the effective barrier height φ_B exceeds slightly the energy gap and is independent of the work function in metal.

Assuming $\varphi_B = E_g$, the expression (8) takes the form

$$(R_0A)_{M\text{-}S} = \frac{h^3}{4\pi q^2 k} \frac{1}{m^* T} \exp\left[\frac{E_g}{kT}\right]. \tag{9}$$

Numerical results of calculations and discussion

The temperature dependence of the R_0A product, defined by the Auger radiative recombination and the depletion layer, was estimated from the formulae (2), (5), and (7). The calculations were carried out for optimum effective doping concentrations for which the R_0A product takes the maximum value. From the calculation performed in the work [13] it follows that, for instance, at the temperatures 77, 200, and 300 K these concentrations are equal respectively to 6×10^{23} m^{-3}, 3×10^{24} m^{-3}, and 1×10^{25} m^{-3}. If this concentration is exceeded an abrupt drop of R_0A occurs, which is caused by the tunnel current. It has been assumed in the calculation that the energy gap in PbTe changes with the temperature in accordance with the formula $E_g(T) = 0.19 + 4.1 \times 10^{-4}\ T$ (expressed in electronovolts) [21]. The effective mass values were determined according to [22], taking the average values of the effective masses of electrons and holes, and assuming that the effective masses change proportionally to the energy gap width. The above approximation is justified by the results of both theoretical and experimental investigations of the band structure of the lead chalcogenide compounds [16, 20]. The values of the effective mass, the anisotropy coefficient K, the carrier mobility μ, the refractive index $\bar{n}$, the static dielectric constant ε_s, and high frequency dielectric constant ε_∞, assumed according to [21, 23], were approximated in the temperature range 77-300 K. The material parameters of PbTe for the chosen temperatures are collected in table. In the calculations of $(R_0A)_{GR}$ it has been assumed that $\tau_0 = 10^{-8}$ s. For lead chalcogenides the time of similar order of magnitudes is often assumed [18, 20].

Table

Material parameters of PbTe

T [K]	$E_g\,[eV]$	m_l^*/m_0	m_t^*/m_0	m_d^*/m_0	m_{tu}^*/m_0	K	$\mu\left[\frac{\mathrm{m}^2}{\mathrm{Vs}}\right]$	$\bar{n}$	ε_s	ε_∞
77	0.22	0.314	0.026	0.037	0.019	12	2.00	6.4	400	38
200	0.27	0.391	0.033	0.047	0.024	12	0.30	6.2	400	36
300	0.32	0.463	0.039	0.056	0.028	12	0.13	6.0	400	34

The results of calculations for the p-n junction are shown in fig. 1. In the temperature of 77 K the main contribution to the current flow through the junction comes from the generation-recombination current of the depletion layer for which $(R_0A)_{GR}$ is the smallest. The theoretical evaluation for the radiative and Auger recombinations give the values greater by four orders of magnitude. As the temperature increases the influence of depletion layer decreases, while in the temperature range above 150 K it is the Auger process which determines the values of R_0A.

The respective calculations for an ideal Schottky junction were carried out by taking advantage of the formula (9) and are represented graphically in fig. 2. In the same figure the temperature dependence of the resultant R_0A of the *p-n* junction, i.e.

$$(R_0A)^{-1} = (R_0A)_R^{-1} + (R_0A)_A^{-1} + (R_0A)_{GR}^{-1}$$

is given for comparison.

From the comparison of the theoretical curves with the experimental data (see fig. 2) it may be seen that a satisfactory consistence has been achieved for *p-n* junction in a wide temperature range. It should be noted that the authors of the works, from which the experimental data have been taken to draw the points in fig. 2, do not report on doping concentrations on both sides of the junction. The experimental values for *M-S* junctions are found only for the temperature of 77 K, deviation from the value calculated for this temperature is very high amounting to four orders of magnitude. This divergence seems to be due to the use of the formula (9) which does not take account of additional processes occurring in the metal-semiconductor junction with narrow energy gap and hole-type conduction. The scheme of energy bands for such a junction has been proposed by Nill and Walpole [20] and is shown in fig. 3, where three regions may be distinguished: inversion, depletion, and bulk ones. In the ideal junction only processes (a), i.e. the hole emission from the Fermi level in metal to the valence band for $h\nu = \varphi_{BC}$ are considered. No account is taken of the excitation of electron-hole pairs in the inversion region (processes (b)), and of the band-band transmissions for electron-hole pairs in the depletion region (processes (c)). The last transitions are of particular importance, because the depletion layer is wide due to high dielectric constant. According to the authors of the work [9] the barrier height φ_{BC} for holes is considerably lowered to take the value φ_{BE} slightly

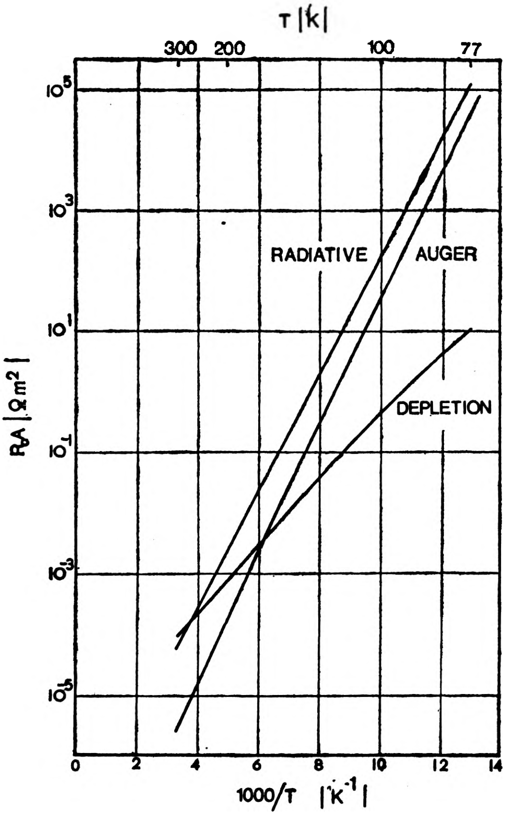

Fig. 1. Temperature dependence of the R_0A product determined by the radiative recombination, Auger recombination and the space charge region for the *p-n* junction

exceeding the energy gap E_g. Since for the holes of kinetic energy slightly exceeding E_g the narrow end of the barrier is transparent due to tunnelling effects, the effective barrier φ_{BE} (determined, for instance, from the *C-V* junction characteristics) is for the majority of metals independent of the working function in metal [12].

The extreme values drawn in fig. 2 for the Schottky junction are comparable with those obtained for the *p-n* junction at

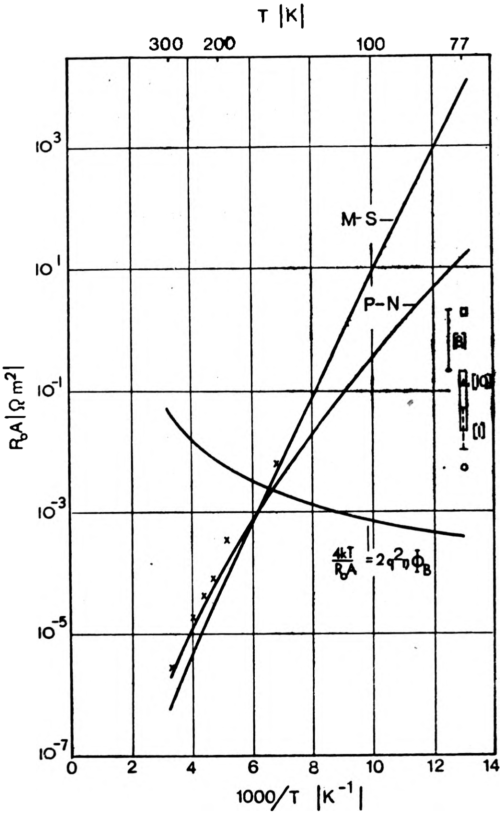

Fig. 2. Temperature dependence of the resultant R_0/A product of the *p-n* junction and an ideal Schottky junction. The experimental points for *p-n* junctions are taken from the papers [1], [4] (□), [7] (×), [8], while those for the *M-S* junctions from the papers: [9] (○), [10], [12] (△)

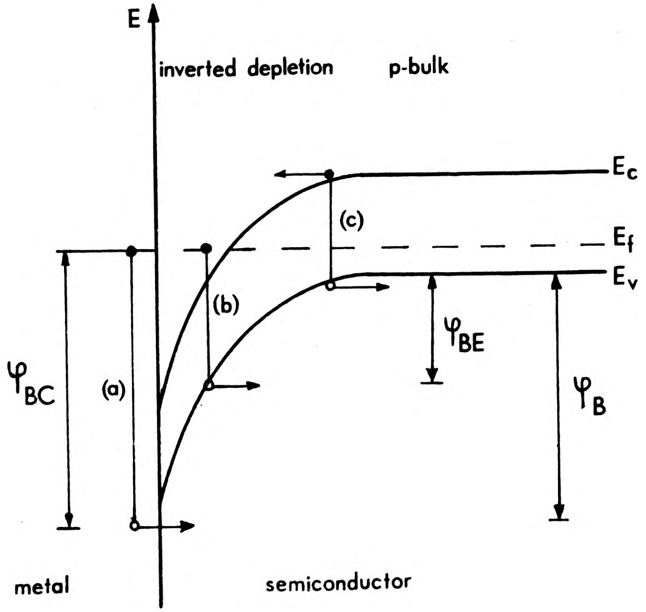

Fig. 3. The energy band scheme for the *M-S* junction with the *p*-type semiconductor with a narrow energy gap (according to [20])

the temperature of 77 K. Since in the last junction the R_0A product is determined by the generation-recombination processes it should be concluded that for the *M-S* junction an essential contribution to the R_0A product comes also from the space charge region. The results reported in [11] may be viewed as confirming somehow this conclusion. There, the authors noticed that Pb-(p)PbSe junctions, at the temperature exceeding 100 K $d(\ln R)/d(1/T) \approx E_g(0\text{ K})/\beta k$, where $\beta \approx 1.8$. The value of the coefficient β is close to 2, which indicates the dominant contribution from the generation-recombination space charge of the junction [19]. Also in the paper [25] it has been stated that the properties of the metal-(p)$Cd_xHg_{1-x}Te$ barrier are determined by the properties of the *p-n* junction rather than by those of the barrier of the ideal Schottky junction.

The operation conditions for the photovoltaic detectors limited by the background radiation (with *p-n* and *M-S* junctions)

The detectivity limited by the Johnson-Nyquist noise of the detector resistance R_0 and the noise generated by the background radiation Φ_B may be determined from the formula [18]:

$$D^* = \frac{\eta\lambda q}{hc}\left[\frac{4kT}{R_0A} + 2q^2\eta\Phi_B\right]^{1/2}, \tag{10}$$

where η is the quantum efficiency, c — light velocity, and λ — wavelength of the incident radiation. This formula is valid for an ideal detector of sensitivity proportional to the radiation wavelength, while the peak of photosensitivity and the long-wave edge of sensitivity are determined by the energy gap width. This formula takes no account of other kinds of noise, such as 1/f. If the background radiation-limited noise is much greater than the Johnson-Nyquist noise (i.e. when $4\,kT/R_0A \ll 2q^2\eta\Phi_B$), the detectivity of detector is limited by the background. In fig. 2 the curve fulfilling the equation $4\,kT/R_0A = 2q^2\eta\Phi_B$ for $\eta = 0.5$ and Φ_B is drawn additionally for the view angle 2π (dependence Φ_B upon the wavelength corresponding to the long-wave edge of sensitivity is assumed to be consistent with that suggested in [26]).

If this curve lies above the resultant curves $R_0A = f(T)$ for the photovoltaic detectors considered, then these detectors do not fulfil the conditions for background-limited operation; if, however, it lies below those curves these conditions are satisfied. The intersection point of these curves occurs at the temperature ~ 150 K. Hence, it follows that for the temperature below 150 K the operation conditions for photovoltaic PbTe detector limited by the background radiation can be easily satisfied. This should not be expected for higher temperature.

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Температурная зависимость произведения R_0A фотовольтаических детекторов PbTe

В работе рассчитаны предельные значения произведения R_0A диффузионных переходов *p-n* PbTe в температурном интервале 77—300 K. Обсуждено влияние диффузионного тока (для излучательной рекомбинации и рекомбинации Аугера), а также генеративно-рекомби-

национного тока на R_0A. Расчёты произведены для оптимальных концентраций примесей при которых участием тоннельных составляющих тока можно пренебречь.

Произведены также расчёты R_0A для перехода Шоттки. Результаты расчётов сопоставлены с экспериментальными данными других авторов. Было получено хорошее соответствие для переходов *p-n*. Предпринята попытка выяснения расхождения для переходов Шоттки. Определены рабочие режимы фотовольтаичных детекторов, обнаруживающая способность которых ограничена фоновым излучением.