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Active region of CdTe X-/γ-ray detector with Schottky diode

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Abstract. It has been shown from the Poisson equation that the presence of deep levels in the semiconductor bandgap influences in a complicated manner upon distribution of the space charge, potential and electrical fields in the Schottky diode. Under high reverse bias, however, the diode characteristics become standard. To achieve semi-insulating conductivity in CdTe, it is impossible to widen considerably the depleted layer in the diode. Therefore, the region of the high electric field is only a small part of the substrate thickness. Too small capacitance value and its weak dependence on the bias voltage observed in the Schottky diode made of semi-insulating CdTe are a result of the effect of the substrate resistance and the wide space charge region in the diode.

Keywords: Cz-Si, hydrogen, helium, implantation, diffusion, high pressure, treatment.

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1. Introduction

Over decades, CdTe has been a major material for semiconductor X-/γ-ray detectors widely used in science, technology, medicine, and other fields. However, the manufacturers of CdTe detectors were faced with a variety of problems. The first problem is related to the short lifetime of current carriers, the second one – to elaborate preparation of homogeneous single crystals with semi-intrinsic electric conductivity. In the early 1990s, it was revealed that technological problems could be overcome more readily by substituting $Cd_{1-x}Zn_xTe$ ($x = 0.05$ to 0.1) alloy for CdTe. However, it did not bring meet with any qualitative improvement of the situation.

As far back as in 1966-1967, broad perspectives for using the Schottky barrier in CdTe X-/γ-ray detectors was discovered [1, 2]. Later on, the repeated attempts were made to create detectors with the barrier structure (*p-i-n*, *m-π-n*) [3, 4]. However, these works ceased to be topical after developing commercial detectors based on homogeneous CdTe single crystals, and next $Cd_{1-x}Zn_xTe$ with characteristics acceptable for practical use. Nevertheless, in the late 1990s, in a number of publications, T. Takahashi *et al.* [5-9] reported the results testifying the exceptionally high performance of CdTe detectors with In/*p*-CdTe Schottky barrier having no special scheme for electric signal processing in a detector circuit [10].

Nevertheless, some important questions concerning the role of the Schottky barrier in these devices and its parameters are unclarified. In this work, analyzed are the key characteristics responsible for detecting capability of such detector type, specifically its active region thickness.

2. Effect of deep levels in the semiconductor bandgap on Schottky diode characteristics

The potential energy $\varphi(x,V)$, field intensity $F(x,V)$, and width of the space charge region $W(V)$ in the Schottky diode are determined using the Poisson equation that has the following form in the one-dimensional case:

$$\frac{d^2\varphi}{dx^2} = \varepsilon\varepsilon_0 Q(x,V)\,, \qquad (1)$$

where $Q(x,V)$ is the space charge density, ε_0 and ε are the free-space and semiconductor permittivities, respectively.

If electric conductivity of *p*-type semiconductor is determined by shallow (totally ionized) acceptors with the concentration N_a, the space charge density can be considered as x independent, and the Poisson equation is solved analytically, while $\varphi(x,V)$, $F(x,V)$, and $W(V)$ are described by the known expressions [11]:

$$\varphi(x,V) = (\varphi_o - eV)\left(1 - \frac{x}{W(V)}\right)^2, \qquad (2)$$

$$F(x,V) = \frac{2(\varphi_o - eV)}{eW(V)}\left(1 - \frac{x}{W(V)}\right), \qquad (3)$$

$$W = \sqrt{\frac{2\varepsilon\varepsilon_0(\varphi_0 - eV)}{e^2 N_a}}\,, \qquad (4)$$

where φ_0 is the barrier height in the equilibrium state, e is the electron charge (the coordinate is measured from the semiconductor surface).

The purest and most perfect CdTe single crystals are known to contain impurities (defects) with the high concentration from 10^{15} to 10^{17} cm^{-3}, including the deep acceptors with different ionization energies [12,13]. In this case, the space charge density is no longer invariant, and the Schottky diode characteristics undergo some qualitative modification.

Let us consider the Schottky diode in a semiconductor comprising three acceptor levels, namely, a shallow level E_{a1} and two deep levels E_{a2} and E_{a3} (Fig. 1). The shallow acceptors are totally ionized, and in the bulk of semiconductor their charge is compensated by holes in the valence band. In the part of the barrier region where band bending is not yet sharp, the space charge remains practically unchanged. As the interface is approached, the deep acceptor impurities have the ionization energy E_{a2} that proves to lie below the Fermi level E_F. The space charge density is increased abruptly and remains unchanged until the third type acceptor level (E_{a3}) prove to be located below the Fermi level, resulting in the next abrupt change of values in the relation $Q(x)$.

The Poisson equation for the Schottky barrier in a semiconductor comprising the deep levels is solved using numerical methods [14]. The concentration of charged acceptors, holes in the valence band, and electrons in the conduction one can be represented as follows

$$N_{ai}^{-} = \frac{N_{ai}}{\exp\left(\dfrac{E_{ai} - \Delta\mu - \varphi(x,V)}{kT}\right) + 1}\,, \qquad (5)$$

$$p(x,V) = \frac{N_v}{\exp\left(\dfrac{\Delta\mu + \varphi(x,V)}{kT}\right) + 1}\,, \qquad (6)$$

$$n(x,V) = \frac{N_c}{\exp\left(\dfrac{E_g - \Delta\mu - \varphi(x,V)}{kT}\right) + 1}\,, \qquad (7)$$

where N_{ai} are the concentrations of acceptors (subscript "i" takes the values 1, 2, and 3), $N_c = 2(m_n^* kT/2\pi\hbar)^{3/2}$ and $N_v = 2(m_p^* kT/2\pi\hbar)^{3/2}$ are, respectively, the effective densities of states in the conduction and valence bands, $\Delta\mu$ is the Fermi level energy distance from the top of the valence band that was found from the condition of electrical neutrality in the bulk of semiconductor (the spin degeneracy factors of all impurities are assumed to be equal to 1). The acceptor ionization energies E_{a1}, E_{a2}, and E_{a3} were taken equal to 0.05, 0.3, and 0.7 eV, respectively, all three concentrations are 10^{16} cm^{-3}. The following boundary conditions were used: when $x \to \infty$ and $x = 0$ the potential energy $\varphi \to 0$ and $\varphi = \varphi_0 =$ = 0.75 eV, respectively.

From Fig. 1, it follows that the foregoing arguments are proved by the results of computer calculations of the space charge density $Q(x)$. Generally supposed in the Schottky diode invariability of the space charge density is absent: three horizontal sections with transition regions between them are distinctly seen in the $Q(x)$ curve.

It is evident that a complicated behavior $Q(x)$ also changes the coordinate dependences of the potential and electric field intensities represented by Eqs (2) and (3). Moreover, in the presence of deep impurities the space charge density becomes voltage dependent, and the Schottky diode characteristics call for a more detailed consideration. The results of calculation of the space charge density and electric field intensity for various voltages are represented in Fig. 2 (a and b).

At $V = 0$, in the layer adjacent to the neutral region of diode structure, the space charge is created only by shallow acceptors, but as the surface is approached, the impurity with the ionization energy E_{a2} and the next E_{a3} becomes involved. On application of the reverse bias, the space charge region is expanded so that the region (where the space charge density is determined by all the impurities (horizontal section)) is expanded "with advance". The latter means that as the voltage increases, the region where the electric field intensity is a linear x function is expanded, which is illustrated in Fig. 2b. Besides, the dashed lines in Fig. 2 (a and b) are used to

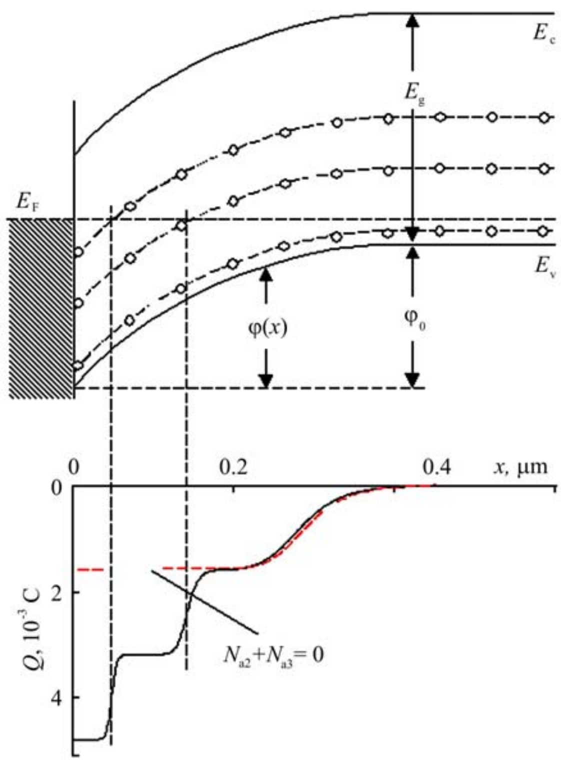

Fig. 1. Energy diagram of the Schottky diode at the equilibrium in semiconductor containing deep levels (at the top). The space charge distribution calculated using the Poisson equation (at the bottom). The dashed line shows the space charge distribution for the case of shallow impurity.

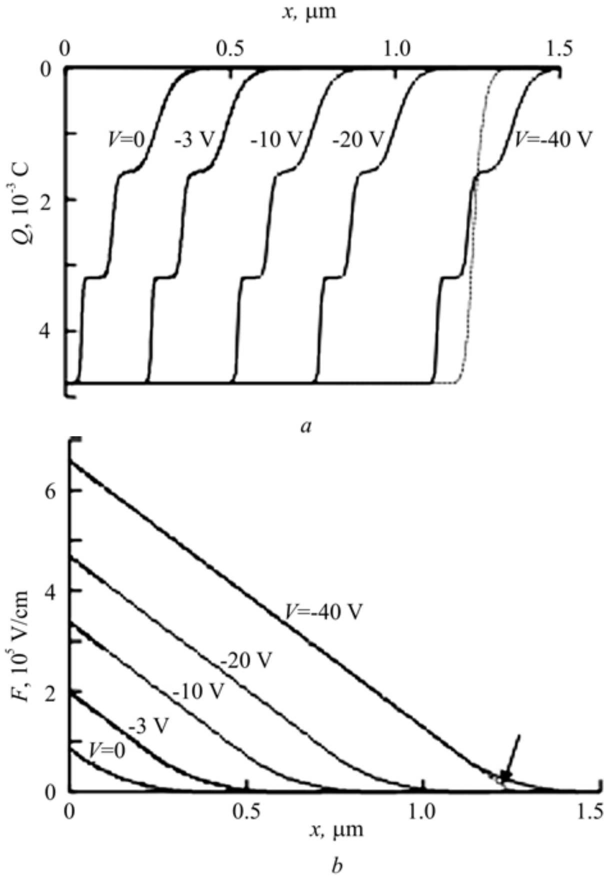

Fig. 2. The space charge distribution in the Schottky diode for a semiconductor with deep levels in the bandgap at various bias voltages (*a*). The dashed line shows the curve calculated for $V = -40$ V for the shallow level with the concentration equal to the total concentration of all three impurities. The electric field strength in the Schottky diode under the same conditions (*b*). The arrow shows the curve analogous to the dashed line in Fig. 2*a*.

show the curves calculated for semiconductor having one shallow acceptor and the concentration equal to the sum of concentrations of all three acceptors. It is seen that with increasing the voltage (in this case, $V = -40$ V), **in the predominant part of the depletion layer,** the diode characteristics for the case of three acceptor impurities and one impurity, but with a total concentration, are closely related. Hence, the potential distribution $\varphi(x,V)$, the field intensity $F(x,V)$, and the width of the space charge region $W(V)$ in the Schottky diode comprising a lot of acceptor impurities at higher reverse bias in semiconductor are described by Eqs (2), (3), and (4), if N_a implies **the total** acceptor concentration.

3. Compensation effect

Preparation of semi-insulating material with a considerable concentration of several acceptor types stipulated above is possible only with their donor compensation. Analysis shows that, to attain near-intrinsic conductivity, 100 % compensation of impurity (defect) determining the material conductivity is not necessary whatever [15].

Let us consider a semiconductor comprising a relatively shallow acceptor impurity with the ionization energy $E_{a0} = 0.1$ eV and a deep acceptor impurity level that can occupy various positions in the bandgap. The position of compensating donor impurity level is of no importance, if it is located several kT above the deep acceptor level (in calculations, the donor ionization energy is assumed to be equal to 0.1 eV). The concentrations of holes and electrons in the bands, as well as of charged acceptors are described by the respective expressions (6), (7), and (5) for $\varphi(x,V) = 0$ (for the time being the neutral part of the diode structure is considered), and of charged donors – by the expression

$$N_d^+ = \frac{N_d}{\exp\left(-\frac{E_g - \Delta\mu - E_d}{kT}\right) + 1} . \quad (8)$$

The Fermi level positions depending on the compensation degree $\xi = N_d / N_a$ are determined from electrical neutrality condition that, for the scheme under consideration, is of the form

$$n + N_{ao}^- + N_a^- = p + N_d^+ . \quad (9)$$

Fig. 3 shows the dependences of the Fermi level energy $\Delta\mu$ (measured, like before, from the valence band top) on the donor concentration N_d calculated for $E_a = 0.5$, 0.75, and 1.0 eV (the concentrations of both shallow and deep acceptors is accepted to be equal to 10^{16} cm^{-3}). As can be seen from the figure, for $N_d < N_{a0}$, the Fermi level is located appreciably lower than the deep acceptor one, but for $N_d = N_{a0}$ is captured by it (the so-called pinning). The Fermi level is strictly coincident with the acceptor one for its 50 % compensation

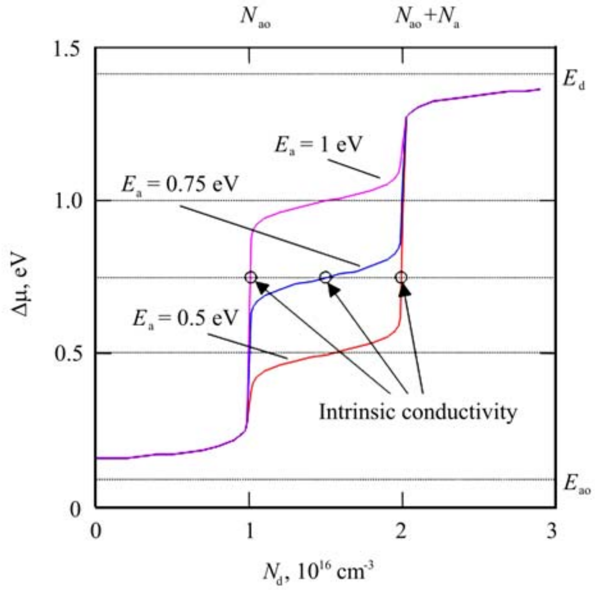

Fig. 3. The Fermi level position as a function of the concentration of the compensating donors for various acceptor depths.

($\xi = 0.5$). As soon as N_d somewhat exceeds the value of $N_{a0} + N_a$, the Fermi level shifts rapidly to the donor level, and semiconductor acquires *n*-type conductivity.

As can be seen, near-intrinsic conductivity ($\Delta\mu =$ $= 0.75$ eV) is achieved in different ways depending on the location of the deep acceptor level. If the acceptor level is located in the middle of the bandgap ($E_a = 0.75$ eV), the intrinsic conductivity is acquired exactly at $\xi = 0.5$, if it is below the middle of the bandgap ($E_a = 0.5$ eV) – at $N_d = N_{a0}$, and if it is above the bandgap ($E_a = 1.0$ eV) – at $N_d = N_{a0} + N_a$. It is important that, in the first case, the point $\Delta\mu = 0.75$ eV lies on the **flat** portion of the curve $\Delta\mu(N_d)$, while in the second and third cases – **on the drastically increasing** portion of the curve. The latter means that, if the compensated acceptor level shifts from the middle of the bandgap, intrinsic conductivity is achieved for the very precise assignment of the compensation degree. At the slightest deviation of the compensation degree, semiconductor conductivity drastically increases due to the increase in electron or hole conductivity component. However, if the compensated acceptor level is located near the middle of the bandgap, the degree of its compensation needs not be met to a high accuracy, and when it varies within $\xi \approx 0.2$ to 0.8, conductivity is relatively little deviated from the intrinsic one. In other words, the easiest way to achieve near-intrinsic conductivity is to compensate the acceptor level located **near the middle of the bandgap**.

From the foregoing, it follows that the concentration of uncompensated acceptors determining the width of the space charge region in the Schottky diode even in the samples with near-intrinsic conductivity cannot be much less than the total acceptor concentration. If, for instance, in the lower part of the bandgap, there are five types of acceptor levels with the identical concentration, for 50 % compensation of the upper level, the concentration of uncompensated acceptors will comprise 1/10 of the acceptor concentration, which will expand the space charge region by a factor of about 3 ($\sqrt{10}$). Moreover, if there are acceptor levels located in the upper part of the bandgap, the effect of compensation on the space charge width will be even weaker.

The foregoing allows us to arrive at a conclusion that the width of space charge region of the Schottky diode W based on compensated semiconductor is of vital importance for the work of X-/γ-ray detector. As was shown above, the value W is determined from Eq. (4) where N_a implies the concentration of uncompensated acceptors. Let us consider how to expand the space charge region through material compensation. The total acceptor concentration is assumed to be $3 \cdot 10^{16}$ cm^{-3}, barrier height is 0.7 eV in the equilibrium state, applied bias voltage $V = -100$ V. Fig. 4 demonstrates the results of calculations of the electric field intensity in the diode for various compensation degrees.

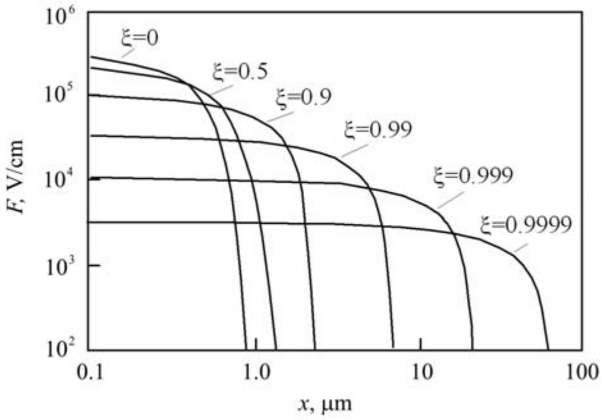

Fig. 4. The electrical field distribution F in the Schottky diode as a function of the compensation degree $\xi = N_d / N_a$ ($N_a = 3 \cdot 10^{16}$ cm^{-3}, $V = -100$ V).

It is evident that, by increasing the compensation degree, one can appreciably expand the diode barrier region. However, to approach 100-μm width the compensation degree has to be of the order of 0.9999 (!). The slightest deviation of ξ from 1 will drastically increase material conductivity. With regard for the present-day technology, to held the compensation degree at such a level and with such a high precision in any extended crystal volume seems to be unreal. The conditions cannot be also much different for the diodes based on semi-insulating material frequently obtained as a result of doping with Cl or other elements (In, V, Ti, Ge, Sn).

Thus, the presence of numerous uncontrolled impurities and defects (10^{15}–10^{17} cm^{-3}) in CdTe single crystals makes it impossible to expand considerably the thickness of the Schottky diode barrier region through material compensation. By assuming, for example, that the acceptor concentration is equal to 10^{17} cm^{-3}, for $\varphi_0 = 0.75$ eV and $V = 0$, we get $W \approx 0.3$ μm. According to the foregoing, semiconductor compensation can increase the barrier region width W no more than several times (W is inversely proportional to the square root of uncompensated acceptor concentration). Thus, at $V = 0$, the width of space charge region does not exceed ~1 μm, and at $V = -(300$ to $400)$ V – several tens of microns (in any case less than ~100 μm). In this respect, the use of compensation (introduction of Cl, In, annealing in Cd vapors) has even negative consequences, since, actually without expansion of depletion layer, the additional doping reduces the lifetime of carriers, and hence aggravates the problem of charge collection.

In the publications [5-9], the electric field intensity in a detector is determined by dividing the applied voltage by the crystal thickness, instead of the Schottky layer thickness. For the diodes in our investigation, this approach is inapplicable, since the width of the depletion layer determined by Eq. (4) is a small part of the crystal thickness and, besides, the electric field distribution in this layer is inhomogeneous.

4. Information from capacity measurements of the diodes

Investigation of capacitance properties allows checking the above results and conclusions, as long as makes it possible to find such critical parameters of the Schottky diode as the potential barrier height φ_0, width of space charge region W, concentration of uncompensated impurities $N_a - N_d$. The dependence of the Schottky diode capacitance on these parameters is described by the known expression [11]

$$C = A\sqrt{\frac{\varepsilon\varepsilon_0 e^2 (N_a - N_d)}{2(\varphi_0 - eV)}}\,, \qquad (10)$$

hence it follows that the dependence of C^{-2} on V is a straight line, and its slope and cut-off on the axes allow determining the above diode parameters.

However, experience suggests that for CdTe Schottky diodes this expression in the majority of cases is not met: the diode capacitance has a weaker dependence on the voltage than it follows from Eq. (10), and the cut-off on the voltage axis yields an absurd value of the barrier height (several electron-volts). As long as the disagreement with the theory becomes more essential for diodes based on high-resistivity CdTe (when the dependence of C on V is not observed at all), one can infer that this is caused by the effect of the substrate series resistance R on the results of capacitance measurements. Because of this, using a conventional resonance method, the scheme of capacitance measurement becomes complicated. Let us consider the effect of resistance R on the resonance frequency, hence, on the result of capacitance measurements.

Fig. 5 (left) shows a scheme for measurements of the diode capacitance C_b. First, the oscillatory circuit is resonance tuned without a diode by means of a calibrated variable capacitor C. For connecting the diode, the resonance condition is met if the capacitance of the capacitor C is reduced by the value of the diode capacitance C_b. Hence, the value C_b is equal to the difference in the above two values of capacitance C.

In a real case, the substrate resistance R is series-connected to barrier capacitance C_b (Fig. 5, right). It is evident that the effect of the diode capacitance C_b on the processes in the oscillatory circuit becomes weaker with

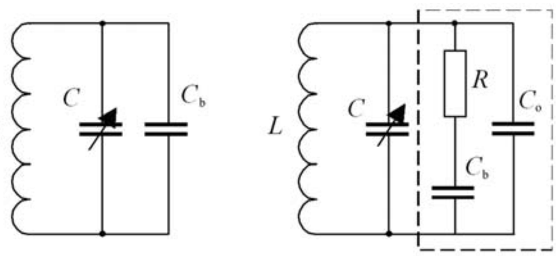

Fig. 5. Circuit for capacity measurements by the resonance method (left). The same with account for the resistance R and capacity C_0 of the substrate (right).

increasing R , and, finally, the capacitance C_0 created by the substrate with two electrodes on the opposite sides becomes dominating. To clear up the conditions for measuring the barrier capacitance or the capacitance of the entire substrate, the impedance of the oscillatory circuit was been found using the scheme shown in Fig. 5 (right), and the resonance frequency has been done by equating the imaginary resistance part to zero.

The diode structure capacitance (shown by the dashed line) is a series-connected capacity resistance $1/i\omega C_b$ as well as an active resistance R. In its turn, the resistance $1/i\omega C_b + R$ is put in parallel with the capacity (resistance) $1/i\omega C_0$. With regard for the series-connected inductive resistance, the impedance can be written as

$$Z = i\omega L + \frac{\dfrac{1}{i\omega(C_o + C)}\left(\dfrac{1}{i\omega C_b} + R\right)}{\dfrac{1}{i\omega(C_o + C)} + \left(\dfrac{1}{i\omega C_b} + R\right)}\,, \qquad (11)$$

$$= \frac{1 + i\omega C_b R}{i\omega C_b + i\omega(C + C_o)(1 + i\omega C_b R)}\,,$$

and for the resonance frequency

$$\mathrm{Im}(Z) = 0\,. \qquad (12)$$

Fig. 6 shows the dependence of Im(Z) on frequency $\nu = \omega/2\pi$ for one of the possible values of R expressed through the material resistivity ρ. In so doing, selected were typical values of the sample thickness $d = 0.1$ cm and the diode area $A = 0.3\times0.3$ cm^2. For given W, d and A, the expressions for the capacitor capacitance are

$$C_0 = \varepsilon\varepsilon_0 \frac{A}{d}\,, \qquad (13)$$

$$C_b = \varepsilon\varepsilon_0 \frac{A}{W}\,. \qquad (14)$$

For L and C selected, the respective real values 0.003 H and $2\cdot10^{-10}$ F. Fig. 6 illustrates a graphical method for solving the equation Im(Z) = 0 (11), when the resonance frequency ν_0 is found at the intersection of the curve Im[$Z(\omega)$] = 0 and the line Im(Z) = 0 (designated by circle). On finding the resonance frequency $\omega_0 = 2\pi\nu_0$, the measured capacitance C_m can be determined as

$$C_m = \frac{1}{\omega_0^2 L} - C\,. \qquad (15)$$

The dependences of C_m on the substrate electric resistivity found in such a manner for several operating frequencies are shown in Fig. 6 (b) (the barrier thickness at zero bias $W_0 = 0.3$ μm, the substrate thickness $d = 1$ mm).

As can be seen, the result of measuring C_m coincides with the diode barrier capacitance C_b only for the low substrate resistivity ρ, whereas for large ρ, the entire crystal capacitance C_0 is measured, which, naturally, does

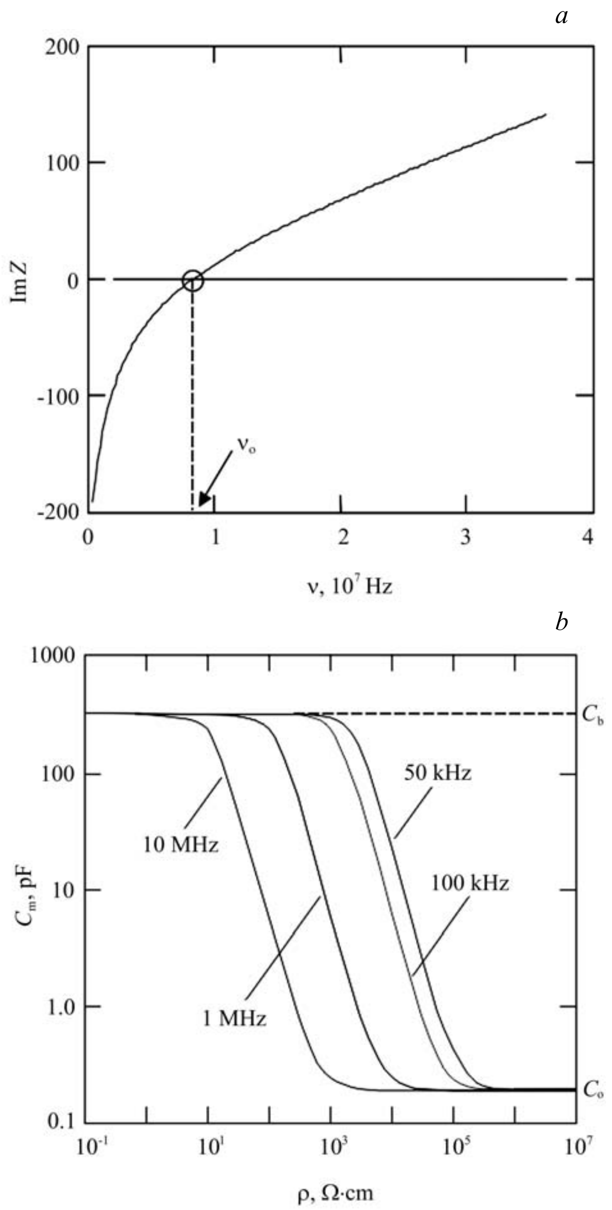

Fig. 6. Graphical method to solve Eq. (11) (a). The measured capacity of the Schottky diode C_m as a function of the substrate resistivity ρ for different frequencies (b).

not depend on the voltage applied to the diode. In a wide frequency range, measurements yield the capacitance values intermediate between C_b and C_0. The true value of C_b can be obtained at the frequency $\nu = 50$ kHz only for the diode with the substrate resistivity $\rho < 10^3$ Ohm·cm. With increasing frequency, the capacity resistance of the barrier region $1/\omega C_b$ is reduced as compared to the resistance R. Therefore, the range of variation in ρ, wherein the measured results give the values of C_b, is narrowed down to $\rho < 1$ Ohm·cm. Hence, too low capacitance values observed for a diode based on the high-resistivity material and its weak voltage dependence is attributable not to large thickness of the space charge region, but to the effect of the series-connected substrate resistance.

5. Conclusions

From solving the Poisson equation for the Schottky diode in semiconductor with deep acceptor levels in the bandgap and their compensation, it follows that the concentration of uncompensated impurity in semi-insulating CdTe cannot be considerably less than the total concentration of all impurities incorporated. This fact, in turn, means that the width of the strong electric field region in the Schottky diode based on semi-insulating CdTe constitutes the minor portion of substrate thickness (not exceeding several tens of microns). Too low capacitance value observed for a diode based on the high-resistivity material and its weak dependence on bias voltage (if any) is attributable not to large thickness of space charge region, but to the effect of the substrate resistance.

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