

SEMICONDUCTOR STRUCTURES, LOW-DIMENSIONAL SYSTEMS,
AND QUANTUM PHENOMENA

Determination of the Parameters of Metal–Insulator– Semiconductor Structures with Ultrathin Insulating Layer from High-Frequency Capacitance–Voltage Measurements

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Submitted December 14, 2017; accepted for publication December 29, 2017

Abstract—A simple numerical method for processing the data of the high-frequency capacitance–voltage characteristics of metal–insulator–semiconductor structures is proposed. The approach is based on analyzing the experimental characteristics near the flat-band states, where the charge exchange of surface localized electron states is of little importance compared with changes in the near-boundary charged layer in the semiconductor. The developed technique makes it possible, first, to find the necessary parameters of the semiconductor and insulating layer and, second, to obtain the experimental field dependences of the energy-band bending in the semiconductor and the total concentration of the built-in charge, the charge of boundary states and minority charge carriers at the semiconductor–insulator interface in the range from the flat bands to deep depletion. The technique is well applicable to structures with an ultra-thin insulating layer. On *n*-Si-based metal–oxide–semiconductor samples with an oxide thickness of 39 Å, experimental approbation of the proposed approach is carried out. The accuracy of the obtained results is 2–3%.

DOI: 10.1134/S1063782619010081

Experimental investigations of the processes occurring in insulating layers and at their interfaces with a semiconductor require the control of changes in the potential and charge reliefs in metal–insulator–semiconductor (MIS) structures. Information about the band bending in the semiconductor, the charge of boundary states, and the accumulation of minority charge carriers near the surface are obtained from the results of measurements of the high-frequency capacitance of the MIS structures on the basis of classic expressions for the potential relief [1]. To process data on the high-frequency capacitance–voltage characteristics (*C–V* characteristics), it is necessary to know the values of the insulating-layer capacitance C_i , the field-electrode area S , and the dopant concentration N_d in the semiconductor near its boundary with the dielectric. The first two quantities are found reasonably easy: C_i coincides with the highest value of the high-frequency capacitance \bar{C} corresponding to the surface charged semiconductor layer and the insulating gap (i.e., in the deep-enrichment region). The variable \bar{C} as a function of the field-electrode voltage V_g is determined directly from the measurement data (see below). The value of S is established from optical measurements. It is more complicated with N_d . First, it is known, for example, for silicon structures [2] that,

in the processes of high-temperature oxidation of the Si surface and purification of the obtained structures, the N_d concentration near the Si–SiO₂ interface may vary as compared to its value in the semiconductor-substrate bulk. These deviations can achieve dozens of percent, which critically affects the results of processing the experimental *C–V* characteristics for the structures with an ultrathin insulating layer. Second, the boundary states are charge exchanged almost up to the states of the semiconductor flat bands in the experiments at room temperature. Therefore, as are shown below, use of the often applied representation of the *C–V* characteristics in the Schottky depletion-layer model with the voltage-independent built-in charge leads to significant errors. Thus, it is necessary to find the dopant-concentration value in a semiconductor directly at its interface with the dielectric and the values of the dimensionless structure parameters calculated on its basis from the measurement data on the field dependences of the high-frequency capacitances of the MIS structures. The calculations should be carried out in the vicinity of the flat-band states, i.e., in the region, where the boundary states are practically filled and barely change their charge with increasing field voltage. In this case, it is difficult to pass to the state of strong enrichment, where the effects of degeneracy and size quantization of the electron system

result in significant deviations [3] of the $C-V$ characteristics from the classical form [1]. This study is dedicated to developing such an approach for determining the values of the parameters of MIS structures from the experimental high-frequency $C-V$ characteristics.

The specificity of samples with an ultrathin dielectric layer of the thickness $h < 50 \text{ \AA}$ consists in the necessity of taking into account at least the resistance of the base when measuring the $C-V$ characteristics [4–6] and conducting experiments under nondestructive conditions, i.e., in a limited voltage range and for reasonably short times [7, 8]. The values of \bar{C} and the conductivity ρ_b of the semiconductor substrate are determined through the values of C_1 and C_2 of the MIS-structure capacitance measured at two high frequencies from the formulas [4, 5]

$$\bar{C} = \frac{C_1 C_2 (\omega_1^2 + \omega_2^2)}{\omega_1^2 C_1 - \omega_2^2 C_2},$$

$$\rho_b = \frac{\sqrt{(C_2 - C_1)(\omega_1^2 C_1 - \omega_2^2 C_2)}}{C_1 C_2 (\omega_1^2 - \omega_2^2)}, \quad (1)$$

where ω_1 and ω_2 are the cyclic frequencies of a variation in the test voltage.

The band bending V_s in the n semiconductor, the total concentration p_{sq} of the built-in charge, the charge of the boundary states, and that of holes at interfaces, expressed in cm^{-2} , are related to the capacitance \bar{C} by the classical relations [1], which in the dimensionless form can be written as

$$\frac{\bar{C}}{C_i - \bar{C}} = \left(\frac{qV_{sh}}{T} \right)^{1/2} \frac{|1 - e^{-v_s}|}{(e^{-v_s} + v_s - 1)^{1/2}}, \quad (2)$$

$$p_{sq} = -\frac{C_i T}{Sq} \left[\frac{qV_g}{T} + v_s + 2 \left(\frac{qV_{sh}}{T} \right)^{1/2} (e^{-v_s} + v_s - 1)^{1/2} \text{sgn} v_s \right], \quad (3)$$

where $v_s = qV_s/T$ is the dimensionless band bending in the semiconductor ($v_s > 0$ with depletion and $v_s < 0$ with enrichment; if we disregard the inequality $V_g|_{v_s=0} \neq 0$, the region $V_g < 0$ corresponds to depletion of the semiconductor, while $V_g > 0$ corresponds to enrichment), q is the elementary charge, T is the temperature in energy units, $V_{sh} = 2\pi\kappa_s q N_d h^2 / \kappa_i^2$, κ_s and κ_i are the permittivities of the semiconductor and insulator, respectively; h is the oxide thickness.¹

¹ It should be noted that the transition layers can occupy more than 40% of the insulator volume in Si–SiO₂–poly-Si structures with a super-thin oxide. Therefore, the values of κ_i and h should be in fact efficient and dependent on the insulator thickness and on the technology of its preparation.

Formula (2) is also valid in the case of the charge exchange of electronic states. Therefore, it is necessary to know the value of the parameter (qV_{sh}/T) for establishing the experimental dependences $v_s(V_g)$ and $p_{sq}(V_g)$.

In the vicinity of flat bands, a range of voltages V_g should exist, where the value of p_{sq} is practically invariable. In this region, we obtain differentiating Eqs. (2) and (3) with respect to V_g

$$\left(\frac{C_i}{C_i - \bar{C}} \right)^2 \frac{2 T d\bar{C}}{\bar{C} q dV_g} = \frac{(e^{-2v_s} + 2v_s e^{-v_s} - 1)}{(e^{-v_s} + v_s - 1)|1 - e^{-v_s}|}. \quad (4)$$

The convenience of Eq. (4) for calculating the parameter (qV_{sh}/T) consists in the direct link between the left-hand side determined from the experimental data and the right-hand side, which is the function of band bending only. Now the procedure for determining the value of the parameter (qV_{sh}/T) can be carried out using successive approximations. At the first step, setting $v_s \rightarrow 0$, we find the voltage V_g corresponding to the flat bands from expression (4). According to the value of the capacitance \bar{C} corresponding to this voltage, we determine the value of the parameter (qV_{sh}/T) from Eq. (2). Using it, we construct the dependence $v_s(V_g)$ from formula (2), and the function $p_{sq}(V_g)$, from Eq. (3). We determine the voltage V_g corresponding to the plateau center on the dependence $p_{sq}(V_g)$ and, already from the dependence $v_s(V_g)$, the value of v_s in the center of the plateau.²

With this value of v_s , we pass to the second step: from Eq. (4), we determine the voltage V_g corresponding to it; from formula (2), we find a new value for the parameter (qV_{sh}/T) ; from relations (2) and (3), we build new dependences $v_s(V_g)$ and $p_{sq}(V_g)$; at the center of the plateau of the function $p_{sq}(V_g)$, we obtain a new value of v_s and pass with it to the next step. The procedure is repeated, until the difference in the values of the parameter (qV_{sh}/T) are within the required accuracy.

The proposed method was experimentally tested in investigations of the MOS n -Si structure with an oxide 39 \AA thick (h is determined from the optical measurements) and the field electrode area of $1.6 \times 10^{-3} \text{ cm}^2$. The $C-V$ characteristics were measured at frequencies of 1 MHz (C_1) and 0.5 MHz (C_2) on a computerized experimental installation [9, 10] using an LCR Agilent

² As the plateau, we should understand a segment of the graph in the depletion region of the semiconductor, where the quantity p_{sq} varies with voltage as weakly as possible. At least, the condition $q|dp_{sq}/dV_g| \ll |dQ_{sd}/dV_g|$, where $Q_{sd} = (2C_i T/qS) \times (qV_{sh} T)^{1/2} (e^{-v_s} + v_s - 1)^{1/2} \text{sgn} v_s$ is the charge per unit area of the semiconductor surface, associated with the overflow of free electrons with changing field voltage should be fulfilled.

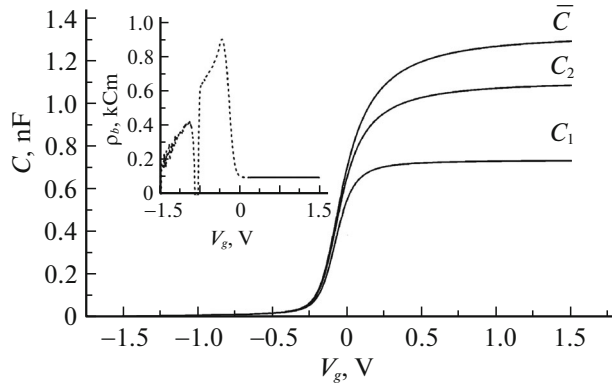


Fig. 1. Dependences $C_1(V_g)$, $C_2(V_g)$, and $\bar{C}(V_g)$, $C_i = 1.303 \times 10^{-9}$ F. In the inset, the dependence $\rho_b(V_g)$ is shown. The dashed line shows the region of an excess in the accuracy measurements.

E4980A precision meter in the dynamic mode: V_g varied with the field-sweep rate $\beta = 16$ mV/s first from 1.5 to -1.5 V (forward branch), then, from -1.5 to 1.5 V (reverse branch). The dependences $C_1(V_g)$, $C_2(V_g)$, and $\bar{C}(V_g)$ are shown in Fig. 1; the forward and reverse branches almost coincide; they are distinguishable only in the region of hole generation [7, 8].

In the inset to Fig. 1, we show the semiconductor-substrate conductivity with variation in the field voltage. The deviation from a constant value occurs only in the region, where, the difference $(C_2 - C_1)$ becomes smaller than the measurement accuracy due to merging of the curves $C_1(V_g)$ and $C_2(V_g)$. The highest value of \bar{C} amounted to 1.303×10^{-9} F; it was taken for the value of C_i . As expected (see Footnote 1),

C_i calculated from this value with the permittivity of the oxide corresponding to a massive sample, the oxide thickness proved to be $h = 42.4$ Å, which is slightly higher than h obtained from the optical measurements.

Table 1. Values of voltages V_g taken for calculating Eq. (4), the dimensionless band banding v_s , and the parameter $(qV_{sh}/T)^{1/2}$ for each iteration

Number of iteration	V_g , V	v_s	$(qV_{sh}/T)^{1/2}$
2	-0.245	1.511	7.323×10^{-2}
3	-0.235	1.158	7.323×10^{-2}
4	-0.224	0.723	7.280×10^{-2}
5	-0.221	0.622	7.258×10^{-2}
6	-0.218	0.483	7.213×10^{-2}
7	-0.213	0.332	7.286×10^{-2}

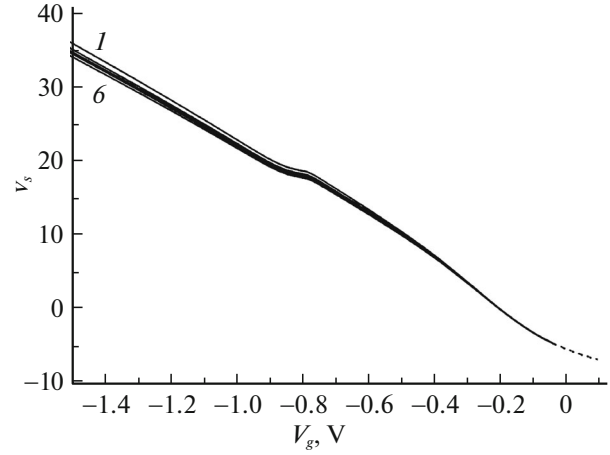


Fig. 2. Dependence of the dimensionless band banding v_s on the field voltage V_g for each approximation. (1–7) are the numbers of iterations; due to the proximity of the curves, the numbers are shown only for the highest (1) and lowest (6) curves. In the region of enrichment, the lines are given by the dashed, line due to mismatch of the used classical technique and the conditions of degeneracy and spatial quantization.

In accordance with the previously described methodology, we made 7 successive approximations. In Figs. 2 and 3, we show the corresponding curves $v_s(V_g)$ and $p_{sq}(V_g)$. At the first step (curves 1), a value of $v_s = 0$ was chosen; it corresponded to the value of $V_g = -0.202$ V in relation (4), and the parameter $(qV_{sh}/T)^{1/2} = 7.413 \times 10^{-2}$ was obtained from expression (2). The data selected further for the calculations as well as the results obtained for the variable v_s and the parameter $(qV_{sh}/T)^{1/2}$ are cited in Table 1; in Figs. 2 and 3; curves 2–7 correspond to them. For the last iteration in the vicinity of the selected voltage V_g , the specific capacitances amounted to as follows: $q|dp_{sq}/dV_g| \approx 9.4 \times 10^{-9}$ F/cm², $|dQ_{sd}/dV_g| \approx \frac{\bar{C}}{S} = 6.6 \times 10^{-8}$ F/cm². From Figs. 2, 3, and Table 1, it follows that the calculation procedure is not divergent, the voltage values selected for the calculations and the resulting values of the variable v_s and the parameter (qV_{sh}/T) are concentrated in small regions around their mean values, the sequence of an increase and decrease in the $p_{sq}(V_g)$ curves as a result of iterations repeats in 6 steps. The values of the parameter (qV_{sh}/T) on the last iterations vary only in the second decimal place. From here, the estimate of the 2–3% error follows. From the value of the parameter (qV_{sh}/T) on the last step, we can determine the value of the dopant concentration in the semiconductor directly near its boundary with the dielectric. If we take the value for the oxide permittivity corresponding to a massive sample (see Footnote 1), it turns out that $N_d = 1.117 \times 10^{15}$ cm⁻³.

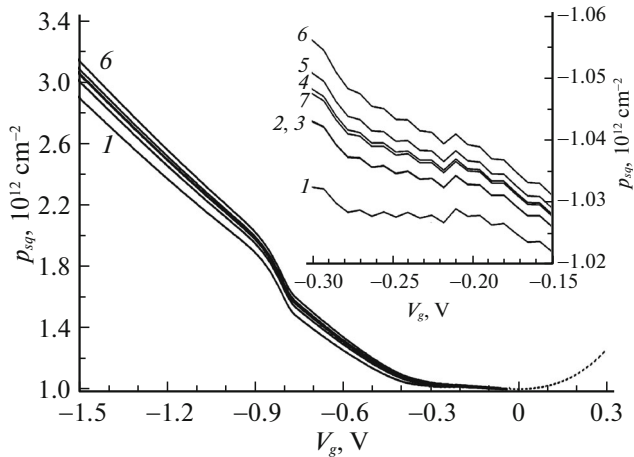


Fig. 3. Dependences $p_{sq}(V_g)$ for each iteration. (1–7) are the numbers of iterations; because of the proximity of the curves, the numbers of only the highest (6) and lowest (1) curves are shown. The dashed line—see the caption to Fig. 2. In the inset, a magnified fragment of curves in the region of voltages, where the parameter (qV_{sh}/T) was calculated, is given.

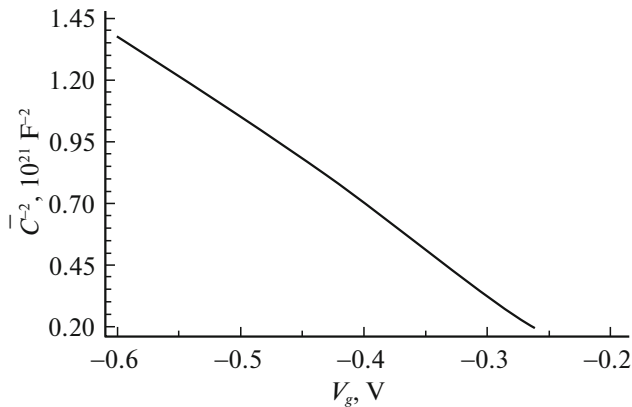


Fig. 4. Dependence $\bar{C}^{-2}(V_g)$ in Schottky coordinates.

It should be noted that the frequently used technique [1] of determining the dopant concentration from the slope of the straight portion of $\bar{C}^{-2}(V_g)$ in the region of $v_s \gg 1$ for high-frequency measurements of samples with an ultrathin insulating layer does not work at room temperature. In Fig. 4, we show the dependence $\bar{C}^{-2}(V_g)$, and the experimental line represents practically the segment of straight line. The value of $N_d = 2.2 \times 10^{12} \text{ cm}^{-3}$ calculated from the slope

of this straight line is absolutely incompatible with the real parameters of silicon substrates.³

Thus, a simple numerical method of processing data on the $C-V$ characteristics for samples with an ultrathin insulating layer at room temperature is presented. The developed techniques makes possible as follows: first, to find the necessary parameters of the semiconductor and the insulating layer; second, in the range from the flat bands to deep depletion, to obtain the experimental field dependences of the band bending in the semiconductor and the total concentration of the built-in charge, the boundary-state charge, and the minority charge-carrier charge at the semiconductor–dielectric interface.

ACKNOWLEDGMENTS

The study was partially supported by the Russian Foundation for Basic Research, project no. 16-07-00666 and within the Programs of Fundamental Research of the Presidium of the Russian Academy of Sciences “Nanostructures: physics, chemistry, biology, fundamentals of technologies”.

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Translated by V. Bukhanov

³ In this region the total concentration of the built-in charge, the boundary-state charge, and the minority charge strongly vary.