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SEMICONDUCTOR STRUCTURES, INTERFACES, AND SURFACES

Depolarization in a Metal–*p*-Ferroelectric–*n*-Semiconductor Structure

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Abstract—The depolarization in a metal–*p*-ferroelectric–*n*-semiconductor structure is calculated based on an analysis of the experimental parameters of a ferroelectric hysteresis loop in a metal–ferroelectric–metal structure. For a semiconductor, the Poisson equation is solved using a standard method, while, for a ferroelectric, a numerical integration is applied. Two variants of semiconductor parameters are considered: (i) a thick *n*-type region (there is a region of electrical neutrality beyond a space-charge region), and (ii) a thin *n*-type region (an electric field penetrates all the way through this region). It is shown that depolarization significantly reduces ferroelectric polarization, and this reduction is stronger in the case of a semiconductor with lower doping. If the electric field penetrates all the way through the *n*-type region, depolarization decreases as the *n*-type region becomes thinner. © *2005 Pleiades Publishing, Inc.*

1. INTRODUCTION

At present, memory elements based on field-effect transistors (FETs) with a ferroelectric gate insulator are being intensively developed (see, e.g., [1–5]). One of the major difficulties encountered when developing FETs is depolarization, i.e., decreasing polarization P in the ferroelectric due to the formation of an opposite charge in a thin semiconductor layer and a voltage drop across this layer. Therefore, analysis of the depolarization in a metal–ferroelectric–semiconductor (MFS) structure and the search for ways to reduce it are currently topical areas of research. Several studies have been devoted to this problem [6–9]. In our own earlier study [10], the hysteresis in a metal–*p*-ferroelectic–*p*-semiconductor was simulated.

In this study, a theoretical analysis of the depolarization and hysteresis in a metal–*p*-ferroelectic–*n*-semiconductor is performed. One example of this kind of structure is the $PbZr_xTi_{1-x}O_3/SnO_2$:Sb structure used in FETs [11–13]. The advantages of these structures are the presence of a *p*–*n* junction, which limits reverse current, and a higher carrier mobility than in perovskite semiconductors.

2. FORMULATION OF THE PROBLEM

A gold layer, forming the Schottky barrier, is deposited onto the ferroelectric, and the contact of the semiconductor to the gold layer is ohmic. In a $PbZrTiO_3$ (PZT) ferroelectric, a passive (blocking) layer, whose thickness d_p is much less than the thickness of PZT [14, 15], can be formed under the gold layer.

Let the voltage drop in the passive layer be negligible; then, the relation

$$V + V_{bi} = \Psi_s + V_f \tag{1}$$

is valid. Here, V is the external bias, V_{bi} is the potential-contact difference between the contact to the ferroelectric and the contact to the semiconductor, Ψ_s is the potential of the semiconductor surface, and V_f is the voltage drop across the ferroelectric.

The inhomogeneity of the ferroelectric was taken into account using the parameters of an experimental hysteresis loop. The inhomogeneity of the semiconductor was considered using the average values of the donor concentration N_d and dielectric constant ε_s. We have assumed that only shallow acceptors are present in the ferroelectric and only donors in the semiconductor, and that defects are located at the interface between the ferroelectric and semiconductor (surface states).

On the interface, the relation

$$-(Q_{sc} + Q_{ss}) = \varepsilon_0 E_f + P(E_f) \tag{2}$$

is valid. Here, Q_{sc} is the charge in the space-charge region of the semiconductor, Q_{ss} is the charge of the surface states, $\varepsilon_0 = 8.85 \times 10^{-12}$ F/m is the permittivity of free space, E_f is the electric field in the ferroelectric, and $P(E_f)$ is the polarization in the ferroelectric at E_f.

We now consider the general case for research using an unsaturated hysteresis loop (Fig. 1). For this situation, we have approximated the $P(E_f)$ dependence with the following expressions [16]:

For an ascending branch,

$$P(E_f) = P_s \tanh\left(\frac{E_f - E_c}{2d}\right) + P_r(1 - a). \tag{3}$$

For a descending branch,

$$P(E_f) = -P_s \tanh\left(\frac{-E_f - E_c}{2d}\right) - P_r(1 - a), \tag{4}$$

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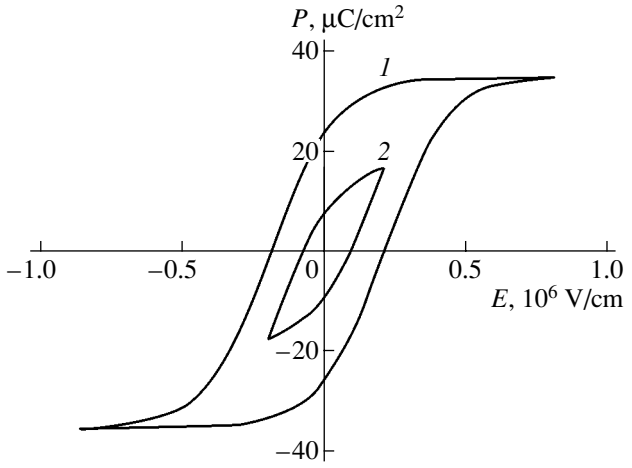

Fig. 1. Hysteresis loops for an MFM structure: (*1*) saturated, $P_s = 35$ μC/cm^2, $P_r = 25$ μC/cm^2, $E_c = 2 \times 10^5$ V/cm; and (*2*) unsaturated, $a = 0.5$.

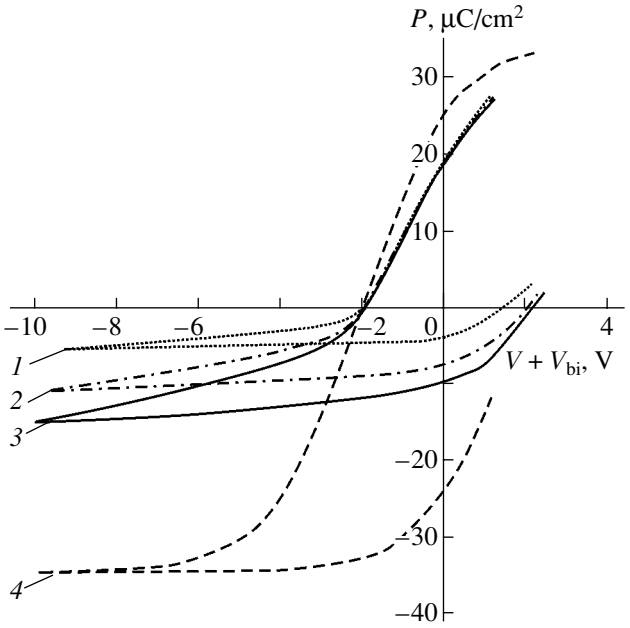

Fig. 2. Saturated hysteresis loops for the metal–*p*-ferroelectric–*n*-semiconductor structure at different donor concentrations ($N_{ss} = 0$). N_d: (*1*) 10^{19}; (*2*) 5×10^{19}; (*3*) 10^{20} cm^{-3}; (*4*) a ferroelectric with the same parameters but without impurities; an MFM structure with $w_f = 1000$ Å.

where P_s is the saturated polarization, P_r is the remanent polarization, E_c is the coercive field, and the coefficient $a \le 1$. At $a = 1$, Eqs. (3) and (4) change into equations for a saturated hysteresis loop [17]. In the calculation of the ascending branch, we use, along with Eq. (3), Eqs. (1)–(3) from [18].

The solution to the Poisson equation for a semiconductor is well known (see, e.g., [19]). For a ferroelectric, the Poisson equation is integrated numerically.

In the calculation, we used the following parameters of the ferroelectric: $P_s = 35$ μC/cm^2, $P_r = 25$ μC/cm^2, $E_c = 2 \times 10^5$ V/cm, the acceptor concentration $N_a = 10^{18}$ cm^{-3}, and the thickness of the ferroelectric $w_f = 1000$ Å. For the semiconductor, we set $\varepsilon_s = 10$, and the concentration of donors N_d is varied in the limits 10^{17}–10^{20} cm^{-3}.

To estimate the effect of the surface states on the shape of the hysteresis loop, we assume that the density of the surface states is constant across the entire width of the band gap. The characteristic time for a thermal emission of electrons from the surface states strongly (exponentially) depends on the ionization energy (see, e.g., [19]). Therefore, we assume that the charge of the surface states has enough time to follow the variation of the external bias for states with the ionization energy E below some critical value E_{cr} and fails to do so for states with energy above E_{cr}. We set $E_{cr} = 0.7$–0.8 eV.

3. CALCULATION RESULTS

We will discuss two possible variants of the semiconductor parameters.

1. The thickness of the space-charge region h is less than the *n*-type region thickness W. This situation is typical of the PZT/SnO_2 structure.

2. The space charge region extends across the *n*-type region as far as the base contact. In the general case, the field on the contact is not equal to zero. This situation can arise in the metal–*p*-PZT–metal structure when an *n*-type region is formed on *p*-PZT during the deposition of the contacts [20, 21].

We now take each case in succession and examine it.

3.1. h < W

Figure 2 shows the calculated dependences $P = f(V + V_{bi})$ for $N_{ss} = 0$ and three values of N_d (curves *1*–*3*). For comparison, curve *4* shows a hysteresis loop for a metal–ferroelectric–metal (MFM) structure with the same parameters of the ferroelectric but without impurities (curve *4*).

When the semiconductor surface is enriched ($\Psi_s > 0$), its properties are close to the properties of metal; therefore, at $\Psi_s > 0$, the portions of the descending branches of the MFM and metal–*p*-ferroelectric–*n*-semiconductor–metal structures are close to each other.

When the semiconductor surface is depleted ($\Psi_s < 0$), an increase in the bias leads to an increase in the magnitude of the semiconductor surface potential. Under such circumstances, the voltage across the ferroelectric and its polarization are only slightly changed. Therefore, the polarization of the metal–*p*-ferroelectric–*n*-semiconductor–metal structure is significantly less than the polarization of the MFM structure. This behavior is more clearly pronounced for semiconductors with

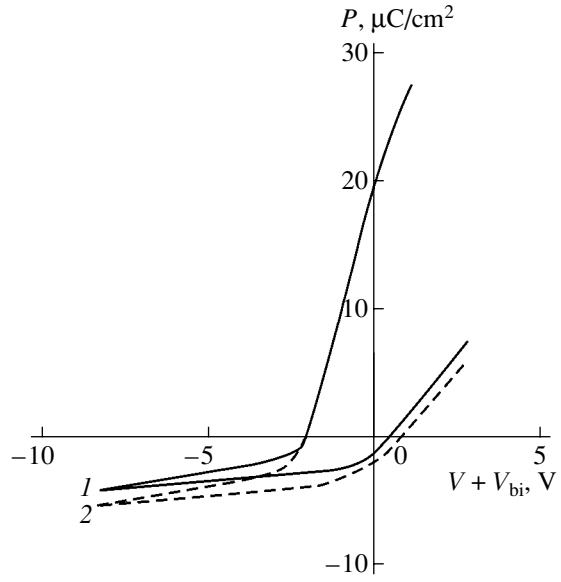

Fig. 3. Saturated hysteresis loops for the metal–*p*-ferroelectric–*n*-semiconductor structure at different densities of the surface states. N_{ss}: (*1*) 0 and (*2*) 10^{13} cm^{-2} eV^{-1}. N_d = 10^{19} cm^{-3}, w_f = 1000 Å.

lower donor concentrations (cf curves *1–3* at a negative polarization). The dependences $P = f(V + V_{bi})$ for metal–*p*-ferroelectric–*n*-semiconductor–metal and metal–*p*-ferroelectric–*p*-semiconductor–metal structures are symmetric; moreover, in both structures, the remanent polarization (all the other factors being equal) has the same order of magnitude (cf the data from [10]). The hysteresis loops for the metal–*p*-ferroelectric–*n*-semiconductor–metal structure are qualitatively similar to the experimental hysteresis loop for the metal–*p*-(triglycine sulfate)–*n*-Si–metal structure [9], which confirms the validity of our method.

The hysteresis loops were calculated for two surface-state densities: $N_{ss} = 0$ and $N_{ss} = 10^{13}$ cm^{-2} eV^{-1} (at $N_d = 10^{19}$ cm^{-3}) (see Fig. 3). At h = 100 Å, the density of the surface states $N_{ss} = 10^{13}$ cm^{-2} eV^{-1} corresponds to the concentration of traps in the space-charge region $N_t = N_{ss}E_{cr}/h = 0.8 \times 10^{19}$ cm^{-3}. As can be seen from the results of the calculation, at $N_t < N_d$, the surface states exert only a slight effect on the parameters of the hysteresis loop.

3.2. h = W

The space-charge region extends across the *n*-type region. In this case, w_f is the thickness of the ferroelectric without an *n*-layer. Figure 4 shows the calculated dependences $P = f(V + V_{bi})$ for $N_{ss} = 0$ and $N_d = 10^{17}$ cm^{-3} at W = 30 and 100 Å. For comparison, the dependence $P = f(V + V_{bi})$ for a case in which the space charge region does not extend across the entire *n*-type region is also shown (see Section 3.1, Fig. 4, curve *3*).

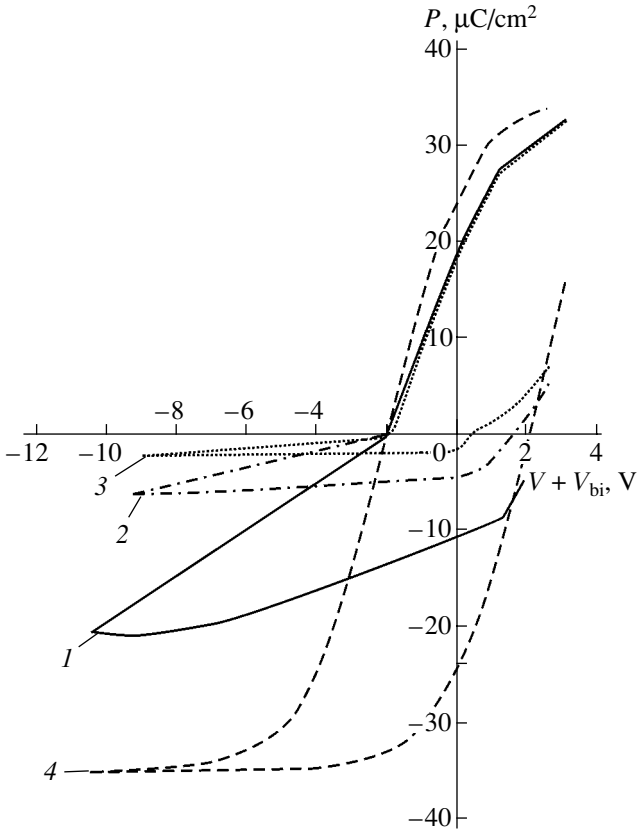

Fig. 4. Saturated hysteresis loops for N_{ss} = 0, w_f = 1000 Å, and $N_d = 10^{17}$ cm^{-3}. *W*: (*1*) 30 and (*2*) 100 Å, (*3*) the space-charge region does not extend all the way through the *n*-type region (for curve *3*, the negative polarization is multiplied by 5), and (*4*) a ferroelectric with the same parameters but without impurities and an *n*-layer.

When the semiconductor surface is enriched, the dependences $P = f(V + V_{bi})$ are close for three values of *W* due to the electron density on the interface approaching the electron density in the metal.

When the semiconductor surface is depleted, the parameters of the structure approach the parameters of the MFM structure without an *n*-layer as the thickness of its *n*-layer decreases. Therefore, as the *n*-layer thickness decreases, the depolarization also decreases (cf Fig. 4, curves *1–3*).

4. CONCLUSION

The depolarization of a metal–*p*-ferroelectric–*n*-semiconductor structure, in which the semiconductor parameters are varied, is analyzed based on the experimental data on a hysteresis loop for an MFM structure.

The Poisson equation for the semiconductor is solved using a standard method, while, for the ferroelectric, a numerical integration is applied.

Two variants of semiconductor parameters were considered:

(i) The thick *n*-type region with a region of electrical neutrality beyond a space-charge region. In this case, the depolarizing effect of the semiconductor leads to a significant decrease in the polarization of the ferroelectric, with this reduction being stronger for a high-resistivity semiconductor. The concentration of the donors in the semiconductor can be estimated from the hysteresis loop in the case of depletion.

(ii) A thin *n*-type region with an electric field penetrating all the way through it as far as the contact. In this case, the depolarization is reduced as the *n*-type region thickness decreases. The *n*-type region thickness can be estimated from the parameters of the hysteresis loop in the case of depletion.

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