Atypical C−V Characteristics of the Al/SmF_3/Ge Structure Caused by Interface and Near-interface Traps

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The existence of near-interface traps, whose energy position is at the same level as the interface states in the middle of the germanium band gap, is proposed as the main factor influencing the atypical $C-V$ characteristics of Al/SmF_3/Ge metal-insulator semiconductor (MIS) structures. These near- interface traps are spatially located in the dielectric very close to the SmF_3/nGe interface and exchange charge with the surface states via tunneling, which helps maintain a high electron density near the interface and create a majority-carrier enrichment regime. When sweeping from positive to negative voltage, the change in the effective charge of the Al/SmF_3/Ge structures was $\sim (4-17)\cdot 10^{-8}$ C/cm^2, which corresponded to a density of near-interface traps of $D_{\text{Nit}} = (5-20)\cdot 10^{12}$ eV^{-1} cm^{-2}.

Keywords: MIS structure, germanium, samarium fluoride, density of interface states, density of near-interface traps, trap capture cross section.

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1. Introduction

The electrophysical characteristics of metal-insulator-semiconductor (MIS) type devices greatly depend on the properties of the gate dielectric layer and the dielectric-semiconductor interface. When a dielectric film is applied to a semiconductor substrate, electrically active defects emerge, localized at the dielectric-semiconductor interface or near it. Given their close proximity to free carriers in the semiconductor, they can effectively capture and release mobile holes and electrons. Defects that can trap or release holes and electrons through thermal emission are known as interface traps (surface states, SS), whereas defects that trap or release holes and electrons through tunneling are called boundary traps (near-interface traps) [1].

Recently, in a number of studies a significant influence of the near-interface traps on variations in electrophysical characteristics of MIS structures (especially in the inversion mode) has been highlighted [1–4]. A change in the experimental quasi-static capacitance-voltage ($C-V$) characteristics of the metal-oxide-semiconductor (MOS) capacitors Al/SiO_2/SiC was observed, which did not exhibit inversion behavior without illumination, but the photostimulated $C-V$-curves showed a capacitance approximately equal to that of the dielectric [2], which was explained by the emission of electrons and holes from traps in the oxide. The presence of boundary traps, together with the quantum confinement effect at SiC/SiO_2 interface, has been proposed as the main factor influencing the field-effect mobility in 4H-SiC-based MOS transistors. These near-interface traps are spatially located in the oxide very close to SiC interface, with a fast response time, with energy levels located at the same level as the conduction band of SiC [1].

Paper [3] covers the study of the near-interface traps in thermally oxidized and annealed in NO SiO_2 films of Al/SiO_2/4H-SiC MOS-capacitors by measuring the transient capacitance. The electrons from the near-interface traps are assumed to first tunnel to the interface traps at the interface, which are at equivalent energy levels, and then they are thermally emitted into the conduction band 4H-SiC. It was found that the filling depth of the near-interface traps is 1.3 nm, which is consistent with the thickness of the non-stoichiometric SiO_2 layer near the interface.

In paper [4], the effects of metal-semiconductor or dielectric-semiconductor interface layers (ILs) in AlGaN/GaN devices were systematically investigated, where AlO_x, TiO_x or NiO_x was used as IL. From the capacitance-voltage characteristics of metal/IL/AlGaN/GaN structures with metal-semiconductor ILs between the gate and AlGaN, it is evident that IL modulates the threshold voltage attributed to the vacuum level jump caused by the fixed charge of IL dipoles.

It is known that high density of interface traps and near-interface traps affects the performance of field MIS transistors, including inefficient modulation of the inversion channel because of a confined trapped charge at the interface and degradation of the effective field mobility in the inversion channel caused by trapping of mobile charge carriers. Therefore, methods capable of quantifying the interface trap density and the corresponding energy position of electrically active defects are crucial for the development of high-quality insulator-semiconductor interfaces to facilitate the use of MIS structures in practice. However, the theoretical basis for explaining the electrical properties and methods for describing the near-interface traps remains unclear and incomplete compared to the

theoretical basis for surface states [3]. In this study we give an insight on the interface and the near-interface traps in Al/SmF_3/Ge structure, which significantly affect the electrophysical characteristics and are responsible for the atypical nature of $C-V$ characteristics.

2. Experimental results

The substrates for MIS structures were the wafers of single-crystal germanium of n-type conductivity GES-2 (111). Samarium fluoride dielectric films were fabricated by thermal spraying of powdered fluoride in vacuum at a pressure of $\sim 10^{-3}$ Pa and temperature of the substrate of $\sim 300\,^{\circ}$C. SmF_3 films exhibit fairly stable and reproducible properties and have a polycrystalline structure. In all cases the thickness of dielectric was 250–400 nm. To obtain MIS capacitances, aluminum electrodes with a diameter of 0.5–0.7 mm were applied to the dielectric using thermal evaporation in a vacuum through a stencil.

To modify the magnitude of the effective charge in the initial dielectric film, the samples were subjected to several cycles of exposure in an environment with high humidity followed by low-temperature annealing. This treatment leads both to a change in the density of surface states and to the creation of new charge centers in the volume of dielectric and in the semiconductor's near-interface region [5,6].

Figure 1 shows the dependences of specific capacitance on the voltage of Al/SmF_3/nGe MIS structure, measured at 1 MHz. The specifics of the experimental $C-V$ in Figure 1 is that at negative voltages, when at a sufficiently high frequency of 1 MHz a drop in capacitance should be observed during implementation of the inversion mode, the high-frequency capacitance-voltage dependences exhibit „low-frequency" behavior. To compare the high-frequency and low-frequency curves, the low-frequency $C-V$-characteristic of an ideal MIS structure with the parameters of GES-2 germanium was calculated (see Figure 1).

The shift in the onset of experimental curve decline relative to the ideal one in the region of positive voltages indicates the presence of a negative charge in the dielectric film. At the same time, a repeated decrease in capacitance, which is already observed in the region of negative voltages, indicates the presence of a positive charge in the dielectric film. Thus, when scanning from positive to negative voltage, the effective charge $Q_f = Q_{ox} + Q_{it}$ changed, which consists of the charge in the dielectric Q_{ox} and the charge of the surface states Q_{it}.

To obtain the dependence of the effective charge variation on voltage $dQ_f(U)$ from the experimental $C-V$-curves, the dependence of the surface potential Φ_S on voltage was calculated. Then, on curve $\Phi_S(U)$, the voltage values U_1 before the minimum and U_2 after the minimum were selected, at which the same values of the surface potential were observed (Figure 2). Since the same values of the surface potential correspond to the same values of the

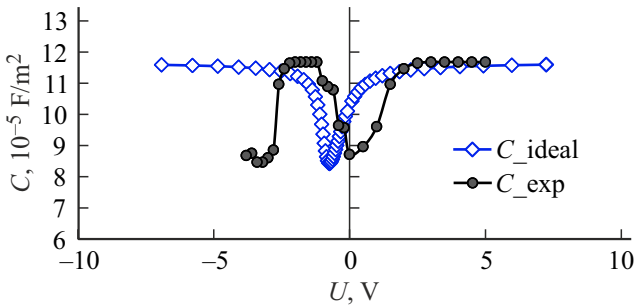

Figure 1. Measured specific capacitance (C_{exp}) of Al/SmF_3/nGe structure at 1 MHz and rated low-frequency ideal specific capacitance (C_{ideal}) versus voltage.

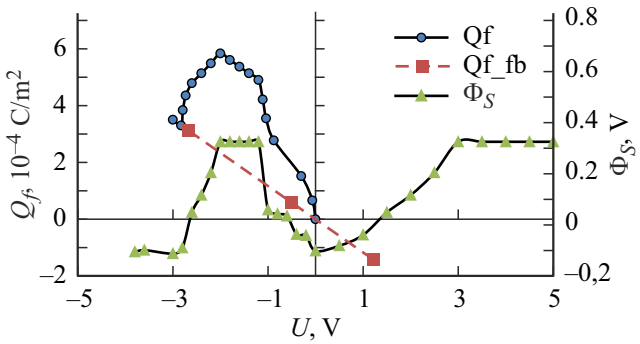

Figure 2. Variations of density of effective charge Q_f and surface potential Φ_S versus voltage of Al/SmF_3/nGe structure.

charge Q_S in the space charge region, we can write

$$U_1 = -\varphi_k + \Phi_S - \frac{Q_{f1}}{C_D} - \frac{Q_S}{C_D},$$

$$U_2 = -\varphi_k + \Phi_S - \frac{Q_{f2}}{C_D} - \frac{Q_S}{C_D}, \qquad (1)$$

where C_D is the specific capacitance of the dielectric, φ_k is the difference in the work functions of the metal-semiconductor, $Q_{f1,2}$ is the specific effective charge in different sections of the surface potential versus voltage curve, Q_S is the specific charge in the space charge region of germanium. Then

$$(U_1 - U_2)C_D = Q_{f2} - Q_{f1}. \qquad (2)$$

The variation of the effective charge versus voltage variation will be written as

$$dQ_f = C_D(U_1 - U_2) = dQ_f(U). \qquad (3)$$

Figure 2 illustrates the curves of the surface potential and effective charge density versus voltage of Al/SmF_3/nGe structure. Higher positive effective charge density is observed with the rise of reverse bias, which was observed for all Al/SmF_3/nGe structures that exhibited „low-frequency" behavior at a frequency of 1 MHz in the inversion mode.

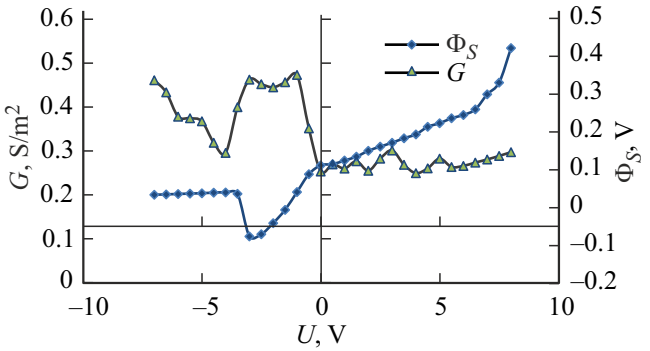

Figure 3. Dependence of the specific conductivity G and surface potential Φ_S on the voltage of Al/SmF$_3$/nGe structure at a frequency of 1 MHz.

The figure also shows the effective charge values Q_{f_fb} obtained from the flat band voltage values (dashed straight line). These dependences prove that the initial effective charge of the structure was negative, and after the surface potential reached the weak inversion mode, the charge becomes positive. The onset of the weak inversion mode in germanium GES-2 corresponds to the value of surface potential $\Phi_S \sim -0.08$ V, in this mode the Fermi level on the surface of the semiconductor is compared with the intrinsic level $n_S = p_S = n_i$, where n_S, p_S is the concentration of electrons and holes on the surface of the semiconductor, n_i is the intrinsic concentration in the volume of germanium. This mode corresponds to bending of bands on the semiconductor surface equal to the difference between the Fermi level and the middle of the band gap in the bulk of germanium $E_F - E_i \approx 0.08$ eV, which leads to the external voltage changing the energy spectrum and causing a controlled redistribution of the electrical density in the system.

The relatively high density of positive effective charge that arose during $C-V$ measurement in the dielectric and at the dielectric/germanium interface for various samples was $\sim (4-17) \cdot 10^{-8}$ C/cm^2. The increase in positive effective charge compensates for most of the negative bias applied to the top electrode, preventing formation of an inversion layer. Therefore, the enrichment layer on the surface of the semiconductor is maintained up to high negative voltages, and the time of the carriers response to the voltage change will be provided by the major charge carriers. This leads to a specific behavior of the capacitance under reverse bias similar to a „low-frequency“ scenario of the capacitance behaviour. However, in this case, when a reverse bias is applied to MIS structure, the capacitance of the dielectric layer and capacitance of layer enriched by major charge carriers on germanium surface are connected in series, and not the inversion layer.

Figure 3 shows the dependences of the specific conductivity G and the surface potential Φ_S on voltage of Al/SmF$_3$/nGe structure at a frequency of 1 MHz, characteristic of some experimental samples. Maximum conductivity is observed near the surface potential value $\Phi_S \approx -0.08$ V, which corresponds to the beginning of the weak inversion mode.

At this value of the surface potential, a recharge of the levels of surface states with an energy of $E_t \sim 0.3$ eV occurs near the middle of germanium band gap, which leads to a higher value of positive charge of the near-interface traps and higher conductivity in the structure. As a result, the surface of the semiconductor goes into accumulation mode, and the surface potential takes on positive values. In the considered case, the corresponding parallel losses are well expressed in $G-V$ curve and tend to grow, which is caused by the exchange of charges between the surface and volume of germanium.

3. Discussion of results

It is assumed that interface traps are spatially located at the semiconductor-insulator interface, where they can easily exchange the charge with the majority of carriers either from the bottom of the conduction band or from the top of the valence band due to thermal emission and carrier trapping. Energetically, these traps form a continuum of energy levels located in the band gap of semiconductor. Traps that are energetically located below the Fermi level are filled, while traps with energy levels above the Fermi level are empty.

In Figure 4, curve *1* is a graph of density distribution of surface states D_{it} by energies in germanium band gap, calculated from $C-V$ characteristics using Terman method. This dependence is quite typical for Al/SmF$_3$/nGe structures, both exhibiting and not exhibiting specific „low-frequency“ behavior at a frequency of 1 MHz. Here, a peak is observed at $(E_C - E_F)_S = 0.3$ eV (for different experimental samples, this value can lie in the range of 0.3–0.33 eV) and a peak at 0.12–0.14 eV (for other samples, this peak can shift or be

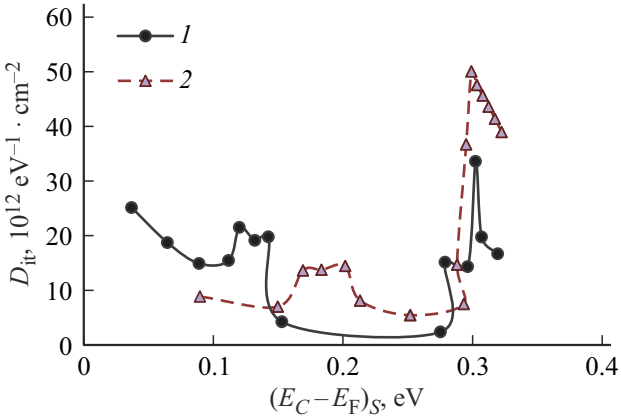

Figure 4. Distribution of density of surface states by energies in the band gap of germanium for Al/SmF$_3$/nGe structure. Here E_C is the energy of the bottom of the conduction band, E_F is the energy of the Fermi level, „S“ index indicates that the parameters belong to the germanium surface.

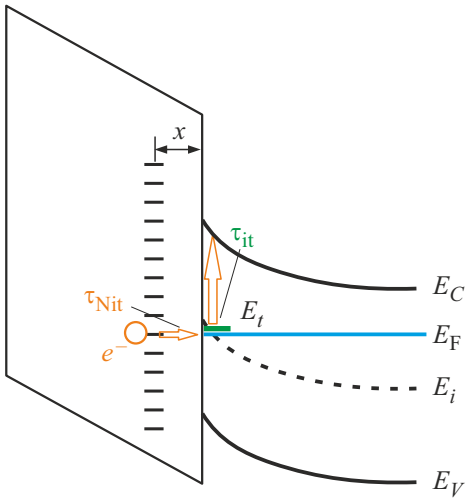

Figure 5. The band diagram of SmF_3/nGe interface in the weak inversion mode, illustrating the process of electron tunneling from the near-interface trap to the $E_t \sim 0.3$ eV energy level of the interface state, followed by a transition to the conduction band of germanium.

absent altogether). The dotted curve *2* represents a similar dependence with a shift of the last peak to the region of 0.17−0.21 eV.

The energy level of 0.3 eV corresponds to the energy value of the surface states E_t approximately in the middle of germanium band gap, as shown in the band diagram in Figure 5, and it is the most intense, i. e., the dominance of this level can be assumed. The shift of energy levels in the range of 0.12−0.21 eV (or their complete absence) indicates that complex microscopic processes can occur at SmF_3/nGe interface.

Figure 5 shows a band diagram corresponding to a „low-frequency" scenario of changes in $C-V$ characteristics at a frequency of 1 MHz. In the absence of an external bias on the field electrode ($U = 0$), the surface can be in the flat band, depletion or enrichment mode; in all these cases, the level of surface states with energy $E_C - E_t \sim 0.3-0.33$ eV lies below the Fermi level. After the weak inversion mode is realized at $U < 0$, the interface traps at $E_t \sim 0.3$ eV, which were previously occupied by electrons, begin to become free (since they will already be located above the Fermi level), and during τ_{it}, electrons from them will move into the conduction band, i. e., create free electrons. After this, the electron concentration in the conduction band rises, and the bending of bands declines, accordingly, the Fermi level approaches the edge of the conduction band on the semiconductor surface, and SS is again filled with electrons, but these electrons already come from the boundary states during the tunneling period τ_{Nit}.

In this mode, the traps can operate for quite a long time, as long as there is a source of electrons from the near-interface traps. After most of the electrons leave the near-interface traps, the structure goes into the strong inversion mode, and „classical" high-frequency behavior is realized in the MIS structure. Thus, interface traps located in the middle of the semiconductor's band gap act as a source for electrons. They capture electrons tunneling from the near-interface traps and then release them into the bulk of the semiconductor. This is consistent with the idea that electrons in the inversion and accumulation layers can tunnel directly both to and from the near-interface traps with energy levels below the Fermi level [1].

The energy position of the near-interface traps levels is difficult to estimate, but based on the speed of their response, it can be assumed that they are at the same, equivalent level with the surface states. The near-interface trap, having donated an electron to an equivalent interface state, can then capture an electron from the boundary state located at a higher energy level, thus ensuring a continuous charge exchange process with the surface states.

The capture cross-section defines the average physically active area of the defect center. If a free electron is located in the vicinity of a defect region, it will have a very high probability of capture. The capture cross-section σ of the interface trap can be found from the trap response time determined by Shockley-Reed-Hall statistics. For n-type substrates, the response time for a trap between conduction band electrons and interface traps can be found as [1]

$$\tau_{it} = \frac{\exp[(E_C - E_t)/kT]}{\sigma \upsilon_{th} N_C}, \qquad (4)$$

where E_C is the bottom of the semiconductor conduction band, E_t is the energy position of the interface trap, σ is the trap capture cross section, υ_{th} is the thermal velocity of electrons, N_C is the effective density of states in the conduction band. Assuming a measurement frequency of 1 MHz, $E_C - E_t \sim 0.3-0.33$ eV, $N_C = 1.04 \cdot 10^{19}$ cm^{-3}, $\upsilon_{th} = 5 \cdot 10^6$cm/s, we obtain a capture cross-section of the interface trap in the middle of germanium band gap $\sigma = (2.1-8.2) \cdot 10^{-15}$ cm^2, which corresponds to the side of a square $\sim (4.6-8.2) \cdot 10^{-10}$ m, i. e. comparable to the size of an atom. The calculated trap capture cross-section with energy levels around the middle of the band gap is quite realistic, this suggests that these traps at a frequency of 1 MHz can participate in the process of electrical conductivity, exchanging charge with the conduction band.

The actual response time of the interface trap may be less than the time inverse to the signal frequency, then the capture cross-section will be larger. It is possible that part of this time is spent on tunneling of an electron from a boundary state, although the tunneling process can occur in parallel, i. e. at a given moment in time, electrons can tunnel to some interface energy levels, and from other, neighboring ones, they can move into the conduction band. The near-interface traps, which are at the same energy level as the interface traps, exchange charge with them and change the threshold voltage from the initial value V_{T0} to V_T. This capture requires a two-step process: electron tunneling from near-surface traps and electron capture by interface

traps. The release time of electrons from the near-interface traps for the tunneling process is usually determined by formula [3]

$$\tau(x, T) = \mathrm{F}(E, T)\tau_0(E)\exp(2Dx), \quad (5)$$

where x is the tunneling distance from the interface, $D = \sqrt{2m^*(E_C^{\mathrm{ox}} - E)}/\hbar$ is the tunneling attenuation coefficient for an electron at the energy level E, E_C^{ox} is the height of energy barrier for tunneling, F is the Fermi-Dirac function, and for τ_0 a wide range of $\sim 0.1-10^3$ ps values is assumed. For example, the assessment showed that maximum distance at which electrons can still tunnel out of SiO_2 layer is 1.4−1.6 nm in $SiO_2/4H$-SiC structure. The maximum tunneling time could be hundreds of seconds, but the minimum time could not be estimated using the aforesaid research method [3].

The near-interface traps density (D_{Nit}) per unit area can be calculated from the trapped charge as follows [1]:

$$D_{\mathrm{Nit}} = \frac{\Delta Q_f}{2kTq}. \quad (6)$$

In equation (6) k — Boltzmann constant, T — temperature, q — electron charge, ΔQ_f — density of effective charge. If we take the change in the effective charge density during the sweep from positive to negative voltage $\Delta Q_f \sim (4-17)\cdot 10^{-8}\,\mathrm{C/cm^2}$, which was observed in the experiment, then the density of the near-interface traps $D_{\mathrm{Nit}} = (5-20)\cdot 10^{12}\,\mathrm{eV^{-1}}\cdot\mathrm{cm^{-2}}$. This is comparable with the density of interface states at the interface, with the minimum density of interface states in the upper half of the band gap being $\sim (2-5)\cdot 10^{12}\,\mathrm{eV^{-1}}\cdot\mathrm{cm^{-2}}$.

Near-interface states, i. e. charged centers in a dielectric near the interface, can proceed from various types of processing, e.g., exposure to a high-humidity environment followed by a short-term annealing [5,6]. The insight on the nature of charged centers at SmF_3/nGe interface, the reasons for their occurrence and stability of their existence are not outlined in this paper.

4. Conclusion

The existence of the near-interface traps with their energy position being at the same level with the surface states in the middle of germanium band gap, is proposed as the main factor influencing the atypical $C-V$ characteristics in MIS-structures of Al/SmF_3/nGe. These near-interface traps are spatially located very close to SmF_3/nGe interface and are characterized by fast response time.

The near-interface states exchange charge with the surface states via tunneling, and this helps maintaining a high electron density near the interface and providing enrichment by the major carriers.

High positive effective charge of Q_f strongly reduces the hole concentration at Ge interface through electrostatic induction, which delays the establishment of the strong inversion mode in Al/SmF_3/nGe structure. The unique positive polarity of Q_f shields the bulk minority carriers from Ge surface, which is beneficial for n-type physical passivation of Ge that can be attained using an electric field.

Conflict of interest

The authors declare that they have no conflict of interest.

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