Influence of deep levels on capacitance-voltage characteristics of AlGaN/GaN heterostructures

J. Osvald[a)]
Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia

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We studied the influence of deep levels in GaN buffer and AlGaN barrier layer on capacitance–voltage characteristics of the AlGaN/GaN structure. Deep level states were assumed to be both donor and acceptor type and were modeled with discrete peak distribution in energy with certain energy distance from the conduction-band minimum for acceptor-type states or valence-band maximum for donor states. For all the cases studied, the presence of the deep levels in the structure influenced mainly the capacitance plateau of the curves and caused the appearance of the capacitance valley. In addition, the deep levels in AlGaN shifted the capacitance curves to more negative voltages, and the deep levels in GaN changed the slope of capacitance decrease after two-dimensional electron-gas depletion. © *2011 American Institute of Physics*. [doi:10.1063/1.3643000]

I. INTRODUCTION

AlGaN/GaN heterostructures are already developed to relatively high levels, but they are still intensively studied in recent years as a basic tool for high-frequency, high-power, and high-temperature active semiconductor devices. But certainly there are still open problems and questions that deserve solutions. One of these is the influence of deep levels present in the heterostructures on their electrical parameters. Deep levels are, in principle, present both in AlGaN and/or GaN layers. Deep levels in GaN and AlGaN layers themselves are in most cases attributed to point defects as Ga vacancies[1] or N vacancies.[2] The most frequently used methods to study their influence on electrical parameters are *I-V* and capacitance–voltage (*C-V*) measurements.[3] Frequency-dependent *C-V* measurement is often used to identify the traps in the heterostructures.[4–6] Among negative effects connected with deep levels, e.g., current collapse is often mentioned. These levels, also named traps, are responsible for carrier trapping/detrapping phenomena. In AlGaN/GaN, high electron mobility transistors (HEMT), the charges moving in and out of the traps on the surface, interface, and/or in the bulk of the heterostructure,[7] influence the density of the two-dimensional electron gas (2DEG) in the channel, causing effects such as current collapse, drain lag, gate and light sensitivity, and transconductance frequency dispersion. In AlGaN/GaN, HEMT current collapse is more pronounced for higher deep acceptor density in the buffer layer because the trapping effects have greater influence. DLTS measurement has shown that the traps are also located at the interface.[8,9] With these interface states a capacitance hysteresis also seems to be connected.[10]

There are practically no studies on the influence of deep levels on *C-V* curves of AlGaN/GaN heterostructures or how these traps influence the capacitance behavior. We tried to analyze the effect of deep levels to be able to differentiate their influence from the effect of other charges on capacitance curves. We explored their influence on *C-V* curves of heterostructures by simulation of electrical transport in such structures.

II. THEORY

We used drift-diffusion approximation for finding out the influence of deep levels on electrical characteristics of the structures. For this purpose, we solved simultaneously Poisson and current-continuity equations. The three equations were solved simultaneously:

$$\begin{aligned}
&\Delta\varphi = -(q/\varepsilon_s)(p - n + N_d^+ + N_a^-) \\
&\frac{\nabla\cdot\mathbf{J}_n}{q} = U, \qquad \mathbf{J}_n = q(-\mu_n n\nabla\varphi + D_n\nabla n) \\
&\frac{\nabla\cdot\mathbf{J}_p}{q} = -U, \qquad \mathbf{J}_p = q(-\mu_p p\nabla\varphi - D_p\nabla p),
\end{aligned} \tag{1}$$

where φ is the electrostatic potential; q is the electronic charge; ε_s is the permittivity of the semiconductor; p and n are the hole and electron densities, respectively; J_n and J_p are the current densities of electrons and holes, respectively; μ_n and μ_p are the mobility coefficients, D_n and D_p are the diffusion coefficients; and U is the net recombination rate. We used the Mayergoyz[11] and Korman and Mayergoyz[12] iterative technique for solving discretized steady-state semiconductor equations. It uses Gummel's block iteration technique for decoupling the Poisson's and electron and hole continuity equations.[13] The result of the solution is the charge concentration and potential curve in the structure. The population of deep levels depends on the position of the Fermi level in the system, and if the structure is not in thermodynamic equilibrium as is the case by current flowing through the structure, it depends on the quasi-Fermi level position. On the other hand, the quasi-Fermi level position depends on the charge state of the deep levels. The probability of the deep level population by two electrons with different spin is determined by the expression

[a)]Electronic mail: elekosva@savba.sk.

$$P(E) = \frac{1}{1 + 2[\exp(E_{DL} - E_{Fn})/k_T]}, \quad (2)$$

where E_{DL} is the deep level energy, E_{Fn} is the position of the quasi-Fermi level of electrons, and 2 is the degeneracy factor.

It is clear that the problem can be solved only iteratively. Another loop must be included into the computational algorithm where this problem is solved. In this loop, we calculate the potential and charge carrier concentration in the situation where the fixed charge of ionized doping atoms depends on external potential. The same procedure was then used for assessment of the influence of deep levels in AlGaN and GaN layers on the *C-V* curves.

We studied the influence of both types of traps: donor-like, which are neutral when occupied and positive if they are empty, and also acceptor states that are neutral when empty and negative when occupied. Donor-like levels are placed in the lower part and acceptor-like traps in the upper part of the bandgap. Deep levels were simulated with discrete peak distribution in energy with certain energy distance from the conduction band minimum (CBM) for acceptor levels and from the valence band maximum (VBM) in the case of donor-type levels.

The deep levels were assumed to be 0.5 eV under the CBM for acceptor-type deep levels. The energy 0.5 eV has the deep level, which has been ascribed in the literature to carbon-related centers in GaN.[14] The same energy difference 0.5 eV but now from the VBM from the symmetry reasons was chosen for studying the influence of donor-type deep levels on *C-V* characteristics (Fig. 1). We also tried to explore the influence of the deep level energy position on the *C-V* curve and we changed the energy distance from the CBM of the deep level to 0.1 eV.

For simulation we assumed AlGaN/GaN heterostructure to consist of a 25-nm-thick AlGaN layer and a 75-nm GaN layer. The layer of GaN was simulated with this thickness because of the limited number of mesh points to obtain reasonable calculation times. Schottky barrier height at the metal/AlGaN interface was set to 1.3 V. The chosen doping concentration of AlGaN barrier layer was 1×10^{18} cm^{-3}. For the GaN buffer layer, two doping concentrations were assumed, and 1×10^{17} cm^{-3} and 1×10^{16} cm^{-3}. For the sheet carrier concentration of 2DEG, we used the value 8×10^{12} cm^{-2}.

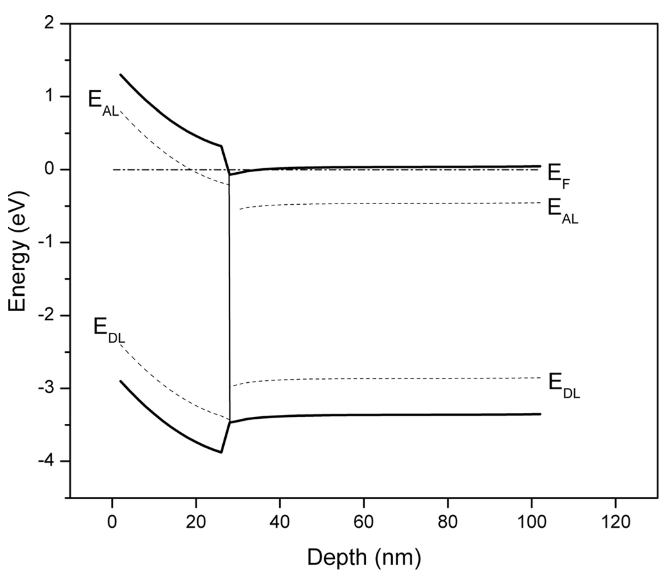

FIG. 1. Energy-band diagram of AlGaN/GaN heterostructure with deep levels assumed in the simulation of deep-level influence on *C-V* curve characteristics.

Because the current is flowing through the structure, and that is why it is not in thermodynamic equilibrium, the population of the states is determined by quasi-Fermi level positions. It is especially true for forward bias where the current is much higher. By the solution of Poisson and drift-diffusion equations, we obtained the potential and carrier concentrations in the whole structure. The simulated *C-V* characteristics were then calculated as

$$C = \frac{dQ}{dV}, \quad (3)$$

from the change of the charge in the structure for two very close voltages. Such calculated *C-V* curves correspond to low-frequency *C-V* curves, because in our calculations we assumed that all free charges are able to respond not only to polarization bias but also to the measuring signal whatever its frequency is.

We note here that it was shown in the literature that relatively high emission constants could be expected at room temperature for deep levels with higher activation energy ($\sim$0.5 eV) in wide bandgap semiconductors,[15,16] and the charge in the traps may not follow even the low-frequency measuring signal. In our study, we want to show how these deep levels can express their presence on *C-V* curves also in this limiting case.

III. RESULTS AND DISCUSSION

We used for our simulations different concentrations of deep levels. To get visible effect and marked change in *C-V* curves, the traps concentration should be in the 10^{16} cm^{-3} order of magnitude. This is practically true for every type of deep level we have studied.

In Fig. 2, the change of the *C-V* curve with increasing concentration of deep levels of donor type in AlGaN buffer layer is shown. For the traps concentration in the 10^{16} cm^{-3} order of magnitude only a small decrease of the capacitance is observed going to forward voltages. This capacitance change is accompanied by a very slight shift of *C-V* curves toward more negative voltages. Marked shift and the capacitance decrease for lower reverse and forward voltages were registered for deep levels concentration 5×10^{16} cm^{-3}. The curves were obtained for GaN doping concentration 1×10^{16} cm^{-3}. The results for 1×10^{17} cm^{-3} were similar.

If there are acceptor-type deep levels present in the AlGaN layer, the simulation shows formation of a valley in the voltage region in which there is approximately constant capacitance for the structures without deep levels (Fig. 3). The depth of the valley is larger for higher traps concentration. We assume that change of the charge state of deep levels shifts the charge centroid and changes effective

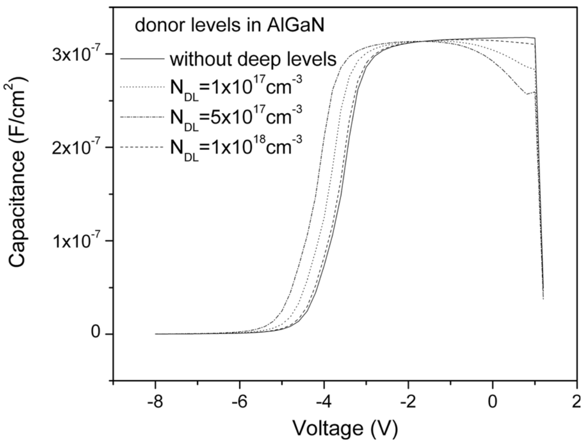

FIG. 2. Influence of the deep donor levels in AlGaN on the *C-V* curve of AlGaN/GaN heterostructure with $N_{AlGaN} = 10^{18}$ cm^{-3}, $N_{GaN} = 10^{17}$ cm^{-3}, and various deep-level concentrations.

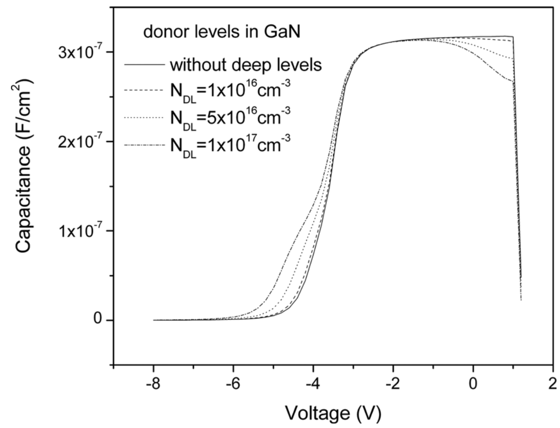

FIG. 4. Influence of the deep donor levels in GaN on the *C-V* curve of AlGaN/GaN heterostructure with $N_{AlGaN} = 10^{18}$ cm^{-3}, $N_{GaN} = 10^{17}$ cm^{-3}, and various deep-level concentrations.

semiconductor depletion layer. The result is the change of the measured capacitance.

The presence of the deep levels of donor type is visible already at lower concentrations in *C-V* curves if the deep levels are situated in GaN buffer layer (Fig. 4). They cause capacitance lowering at lower negative voltages as is the case for deep levels in AlGaN layer, but a new feature in the *C-V* curves is a change of the slope of the capacitance decrease when the depletion of the GaN starts. The capacitance decrease connected with starting of the GaN depletion is not so steep for higher traps concentration because donor type traps under the CBM located near the AlGaN/GaN interface are populated. They diminish the concentration of free electrons in the region, there are fewer electrons that could react to the measuring signal, the capacitance is lower, and the structure behaves like "less" doped. The curves for higher GaN doping concentration are little different. There are two different slopes of the capacitance decrease seen compared to the sample with lower GaN doping concentration. The same effect was observed for the GaN doping concentration-dependent *C-V* curves without the deep levels.[17]

The effect of acceptor-type deep levels in GaN is very similar to the one caused by the deep levels present in AlGaN. In Fig. 5, the formation of the capacitance valley is seen, but now it is more expressed already at lower deep levels concentration. We did not observe any shifting of the *C-V* curves for this type of trap.

We also studied the influence of the energy position of the deep levels on the *C-V* curve. In Fig. 6, two different *C-V* curves for deep donor levels in GaN are shown where the energy distance from the VBM is 0.1, and 0.5 eV, respectively. The capacitance decrease going to the forward voltages appears to be higher for the structures with more deep levels, which are energetically farther from the CBM. We found no influence of the deep level energy on the slope of the capacitance decrease for the case of the deep levels in GaN layer.

Because the shallow doping concentration for AlGaN was also higher than the one for GaN, the concentration of the deep levels had to be higher for AlGaN to cause a visible effect on this higher charge background.

Our results show an interesting feature at lower negative and even positive voltages. The capacitance is not approximately constant with slow decrease, but we obtained a valley in the curve. Going from negative voltages capacitance having reached its maximum, it slowly decreases and then increases again at high forward voltages.

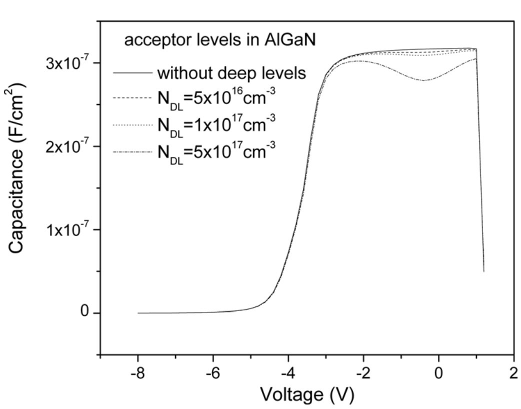

FIG. 3. Influence of the deep acceptor levels in AlGaN on the *C-V* curve of AlGaN/GaN heterostructure with $N_{AlGaN} = 10^{18}$ cm^{-3}, $N_{GaN} = 10^{17}$ cm^{-3}, and various deep-level concentrations.

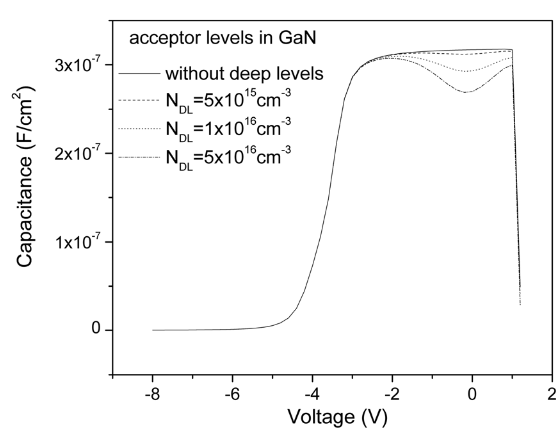

FIG. 5. Influence of the deep acceptor levels in GaN on the *C-V* curve of AlGaN/GaN heterostructure with $N_{AlGaN} = 10^{18}$ cm^{-3}, $N_{GaN} = 10^{17}$ cm^{-3}, and various deep-level concentrations.

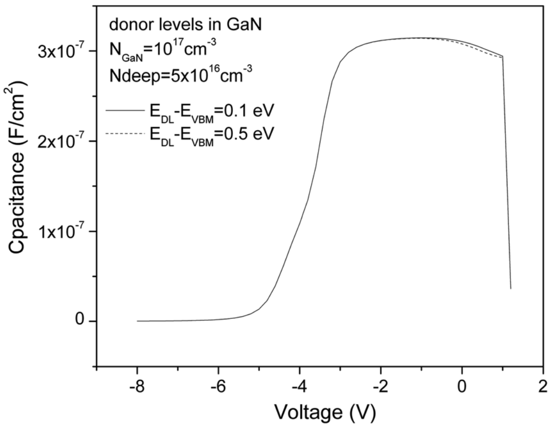

FIG. 6. Dependence of the energy position of the deep level on the *C-V* curve for AlGaN/GaN heterostructure with $N_{AlGaN} = 10^{18}$ cm^{-3} and $N_{GaN} = 10^{17}$ cm^{-3}.

Wang *et al.*[4] measured frequency dependence *C-V* curves of Au/GaN Schottky diodes and found formation of a capacitance peak with the decreasing frequency. They attributed it to the presence of deep level centers. Decreasing capacitance toward forward voltage was observed also by Si *et al.*,[18] which is also probably caused by forming deep levels in the heterostructure by fluorine plasma treatment. Similar capacitance behavior−capacitance peak in the left part of expected capacitance plateau has been observed by Kordoš *et al.*[19] and Irokawa *et al.*[20] But in those experiments, the capacitance plateau was still present in very low negative or even positive voltage. Our results are a bit different from these two. We have not observed such a peak in our simulations. The difference between the published experimental results and the curves from our simulations is the fact that we have practically not obtained the capacitance plateau. The curves with the capacitance peak on the left-hand side of the capacitance plateau were not observed in experimental structures if the capacitance is measured at 1 MHz, the frequency normally used for *C-V* characterization, but for lower measuring frequencies around 1 kHz, which is a witness of deep levels presence.

From our simulation, it cannot be simply stated that the deep levels situated in GaN layer influence more the capacitance in reverse bias and the deep levels in AlGaN layer in forward bias.[21] For example, the effect of deep acceptor levels in AlGaN layer is very similar to the effect of deep levels in GaN layer, only the sensitivity of the *C-V* curves for the deep levels present in GaN is higher than in AlGaN barrier layer.

It is necessary to stress again that the capacitances were calculated at the conditions when all mobile charges are able to follow external measuring signal, i.e., we simulated low-frequency capacitance. Because the emission rates are low and capture times of deep levels are long, predicted curves can be observed on experimental samples only for low measuring signal frequencies and probably could not be expected to appear for measuring frequency ~1 MHz.

IV. CONCLUSION

We have studied the influence of deep levels on the shape and behavior of the *C-V* characteristics of AlGaN/GaN heterostructures. It was shown that the presence of deep levels causes, for all types of deep levels, diminishing of the capacitance for the voltages where there is a capacitance plateau in the case of the absence of deep levels. For donor-type deep levels in GaN, the tilting of the capacitance decrease after the 2DEG depletion was found and may be expected in experimental structures. For donor-type levels in AlGaN, the shift of the *C-V* curve toward more negative voltages is predicted, which is more pronounced for higher deep levels concentration. Finally, we have shown that the deep levels presence in the AlGaN/GaN heterostructures could be at certain conditions—relatively high deep levels concentration and low-frequency measuring signal—detected by standard *C-V* measurement.

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