Extended analysis of the frequency dependence of the admittance of MIS structures with pulsed-laser-deposited AlN films

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Abstract. MIS structures with AlN films deposited on p-Si by pulsed laser deposition were prepared and admittance measurements were carried out in the frequency range of 100 Hz - 10 MHz. The density of traps in the AlN film and at the AlN/Si interface was evaluated using the electrical characteristics obtained, and the hopping mechanism of charge transport was determined from the dispersion of the a.c. conductance.

1. Introduction
Thin films of AlN on Si appear promising as microelectronics components thanks to their high dielectric constant and thermal conductivity, thermal and chemical stability, and good lattice match with SiC and GaN. Still, the potential of AlN as a dielectric has yet to be fully proved. Deposition by rf sputtering [1] and molecular beam epitaxy [2] have so far led to formation of AlN films with high defects concentration, which are responsible for significant leakage currents even at room temperature. Alternatively, pulsed laser deposition (PLD), which has lately become an established method for thin film synthesis, can be used for AlN growth. Its advantages have been demonstrated in many instances where PLD films compared favourably with films produced by other methods.

The AlN-Si structure is a cornerstone for MISFET, memory, sensor and optoelectronics applications of AlN. Preparing AlN-Si MIS structures with low density of deep level traps in AlN and of defects at the AlN/Si interface is an indispensable step towards the utilization of AlN potential. Measuring the capacitance-voltage characteristics and admittance of MIS capacitors at different frequencies is a common method for characterization of deep levels and interface traps in the structures. The admittance technique has an advantage over other techniques such as DLTS due to the extended range of frequencies for deep levels characterization.

In this paper we report the results of our extended analysis of the admittance frequency dependence of MIS structures with pulsed laser deposited AlN films. The density of trapped charges at the AlN-Si interface and the traps in the AlN films are evaluated.

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2. Experimental details
AIn films were prepared by pulsed laser deposition on p-type (100)Si substrates. After loading the substrates and targets, the chamber was evacuated to $5 \times 10^{-4}$ Pa residual gas pressure and the substrates were heated up to 800°C for 1 hour to decompose the native SiO$_2$ covering the wafers [3].

This temperature is sufficiently high to promote the crystalline growth of AlN layers [4]. During the deposition, the polycrystalline AlN (99% purity) target was rotated at 0.3 Hz to avoid piercing.

The target-substrate distance was 4 cm. The deposition was performed by applying 20,000 laser pulses generated by an UV KrF* laser source (248 nm, 7 ns) operating at 2 Hz repetition rate and an energy of 85 mJ/pulse. The film thickness ranged between 600 and 800 nm, which was suitable for the subsequent optical characterization. The ambient nitrogen pressure was kept at 0.1, 5 or 10 Pa.

For the capacitance-voltage (C-V) and conductance-voltage (G-V) measurements, metal-AIn-silicon capacitors were formed by vacuum evaporation through a metal mask of Al dots (1.96x10$^{-3}$ cm$^2$) on the AIn surface. A continuous Al film was evaporated on the Si wafer backside. The admittance measurements were carried out with Tesla impedance meters BM 507 and BM 508 in the range of 1–500 kHz and 500 kHz–10 MHz, respectively, and with a digital LCR meter E7-12 at 1 MHz. The impedance meter simultaneously measured the impedance amplitude, $|Z|$, and the phase angle, $\phi$. These quantities were measured at each frequency with placing the AlN MIS structure in the sample holder ($Z_m$, $\phi_m$) and without it ($Z_a$, $\phi_a$). The impedance of the AlN structure $Z_{AlN}$ and the residual impedance $Z_{in}$ were in parallel to each other. Thus the admittance of the AlN MIS structure, $(Z_{AlN})^{-1}$, was equal to $1/Z_{AlN}=1/Z_m-1/Z_{in}$. The conductance, $G_{AlN}$, and capacitance, $C_{AlN}$, were calculated from $G_{AlN} = \cos \phi_m |Z_m| - \cos \phi_a |Z_a|$ and $C_{AlN} = \{1/\alpha\} \{\sin \phi_m |Z_m| - \sin \phi_a |Z_a|\}$.

3. Results and discussion
The C-V characteristics showed that all Al/AIn/Si structures had the typical behavior of an MIS capacitor, with accumulation, depletion and inversion regions [3]. In figure 1a C-V curves of MIS structure with 760 nm thick AlN film deposited at 0.1 Pa are presented, which were measured at different frequencies and temperatures. The slight decrease of the capacitance measured at 1 MHz in the accumulation region below −6 V is caused by the in-series resistance of the Si bulk, which was estimated to be 125 $\Omega$. The decrease of the capacitance in the inversion region is a manifestation of deep depletion in these AlN MIS structures. Since this effect is more pronounced at 300 K than at 77 K, this suggests that the generation of the inversion electrons at the AlN/Si interface takes place by some non-thermally activated processes. The 1 MHz C-V curve recorded at 300 K is shifted towards more positive voltages in comparison to the ideal one. The shift corresponds to negative built-in charge in the AlN film with a density of 1.8x10$^{11}$ cm$^{-2}$. This comparatively low density of fixed charges can be further reduced by annealing in oxygen ambient [5], so from this perspective, PLD AlN films could appear as good dielectric layers for silicon microelectronics applications. The shift of the C-V curve to more negative voltages at 77 K than that of 300 K indicates the presence of donor-like interface traps. These traps are neutral at 300 K and become positively charged at 77 K due to the Fermi level shift toward the Si valence band by decreasing the temperature. Such donor-like electron traps are also observed in SiO$_2$/p-Si structures [6].

Using the capacitance $C_{max}$ values in accumulation, one can calculate the film dielectric constant.

As it is seen on figure 1a, $C_{max}$ changes with the frequency and, hence, $\varepsilon_{AlN}$ is also frequency dependent. The $\varepsilon_{AlN}$ value, calculated from the 1 MHz curve, is $22\varepsilon_0$ and it is higher for 159 and 15.9 kHz. Similar frequency dependence of the dielectric constant is observed for other AlN/Si MIS structures; it can be explained by the contribution of nitrogen vacancy dipoles to the value of $\varepsilon_{AlN}$ [7].

As the frequency was decreased from 1 MHz to 159 kHz, the $C_{max}$ value increased considerably, while a further decrease of the frequency to 15.9 kHz resulted in a slight increase in $C_{max}$. The change in the $C_{max}$ value as the test voltage frequency is varied is due to the presence of interface traps that are able to charge and discharge at lower frequencies. The difference $\Delta C_{max}$ is a measure of the density $N_{it}$ of these interface traps. This density $N_{it}$, as estimated from $N_{it}=\Delta C_{max}/q$, is within (3-5)x10$^{10}$ cm$^{-2}$eV$^{-1}$ and it is almost constant in that region of the Si gap which is scanned by the Fermi level at the AlN/Si
interface during the voltage sweep from accumulation to inversion. Regardless of the fact that traps with time-constants $>10^{-5}$ s might contribute to a further increase of $N_t$, such a low density of interface traps in a wide region of Si gap sustains the possibility of using AlN as a dielectric layer in Si-based structures.

![Graphs of C-V and G-V characteristics for a MIS structure with an AlN film deposited at nitrogen pressure of 0.1 Pa.](image)

**Figure 1.** C-V (a) and G-V (b) characteristics for a MIS structure with an AlN film deposited at nitrogen pressure of 0.1 Pa and measured at different test frequencies and temperatures. The ideal C-V curve is given by the dashed line. For 1 MHz C-V curves, the solid lines represent the corrected C values with the in-series resistance of Si bulk.

A peak in the depletion region is observed in the G-V characteristics measured at 1 MHz (figure 1b). The density of interface traps as estimated from this peak is $6.9 \times 10^{11} \text{cm}^{-2}\text{eV}^{-1}$. The increase observed of the conductance in the forward-mode as the test frequency is increased is evidence for the influence of the deep levels on the conductance of the structures studied [8]. To clarify this influence, the admittance of the AlN/Si structures was measured at zero DC voltage over a wide frequency band of the AC test voltage (100 Hz - 10 MHz). The results revealed that up to 4 kHz the AC capacitance ($C_{AC}$) of the Al/AlN/Si structures had different behavior when the nitrogen pressure was varied during deposition (figure 2). The $C_{AC}$ of the structure with the AlN film deposited at 0.1 Pa appeared above 5 kHz and further depended only slightly on the frequency (due to the $C_{AC}$ scale this cannot be seen in figure 2). The lack of a pronounced frequency dependence is an indication for a low concentration of deep levels in this AlN film. As for the other MIS structures with AlN films deposited at 5 and 10 Pa, a clear frequency dispersion was observed below 4 kHz (figure 2). For 10 Pa, $C_{AC}$ increased with decreasing the frequency below 4 kHz. This can be explained with the presence of deep traps having time constants higher than $9.1 \times 10^{-4}$ s that contribute to the capacitance at lower frequencies. The density of these traps, estimated from $N_t = \Delta C_{AC}/q$, was $1.2 \times 10^{13} \text{cm}^{-2}\text{eV}^{-1}$. For the films obtained at 5 Pa, the $C_{AC}$ values were negative below 4 kHz, i.e. the phase angle $\varphi$ of the impedance was positive. Such negative capacitance has been detected in other MIS structures [9, 10] and has been attributed to processes connected with electron injection through interface traps.

Figure 3 shows the dependence of the AC conductance ($G_{AC}$) of the AlN/Si structures on the test voltage frequency in the range of 100 Hz - 10 MHz. For the films deposited at 5 Pa, the $G_{AC}$ value was independent of the frequency below 5 kHz, and its value was close to the corresponding DC conductance value [3, 8]. In the case of AlN films deposited at 10 Pa, the conductance was proportional to the frequency in the range 2 - 30 kHz. Such proportionality has been reported for frequencies up to 10 kHz for thermally grown SiO$_2$ films [13]. For 0.1 Pa, $G_{AC}$ appeared above 60 kHz, as in this structures the lowest DC conductance was also observed [8]. Above 60 kHz, $G_{AC}$ increased significantly for all structures, which can be associated with the carriers transported through the structure by a hopping mechanism [11, 12].
4. Conclusions

The extended analysis of the admittance frequency dependence of the MIS structures using pulsed laser deposited AlN films revealed a low trap density at the AlN/Si interface and the presence of deep levels with densities in order of $10^{13}$ cm$^{-2}$eV$^{-1}$ in the AlN films. These levels were responsible for the frequency dispersion observed of the AC conductance through the Al/AlN/Si structure and they contributed to the carrier transport process.

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