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The deep level influence on the admittance of AlN/Si structures with pulsed laser deposited AlN films♣

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The capacitance-voltage characteristics of MIS structures with pulsed laser deposited AlN films have been measured in the 1–20 MHz test voltage frequency range. The results showed an increase of the capacitance in the accumulation regime and the dielectric constant of AlN films, with decreasing test frequency. Such a capacitance increase is larger in AlN/Si MIS structures with higher deep level concentrations in the AlN film.

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1. Introduction

Thin films of AlN, because of their high dielectric constant and thermal conductivity, thermal and chemical stability and fine lattice match with SiC and GaN, are used as insulating layers in various microelectronics applications. AlN films, prepared by different deposition methods, have been investigated from the point of view of their possible applications as gate dielectrics in an AlN/Si MISFET [1], an AlN/Si MIS capacitor sensor for hydrogen [2] and Al/AlN/Si MIS structures with promising applications for program-erasable memory devices [3]. Preparation of AlN-Si structures with a low density of deep level traps in AlN and defects at the AlN/Si interface is a crucial, indispensable step towards the utilization of the AlN potential in the envisaged applications. Depositions by rf sputtering [4] and molecular beam epitaxy [5] have so far led to AlN films with a high concentration of defects, which are responsible for significant leakage currents even at room temperature. One of the recently developed deposition methods is pulsed laser deposition, (PLD). The advantages of pulsed laser deposition (laser ablation), are a congruent evaporation of the AlN target, a high deposition rate, a comparatively low substrate temperature during the deposition and the possibility to deposit stoichiometric AlN films [6].

The investigation of the MIS structure admittance as a function of applied voltage is a powerful method for the establishment of the electro-physical properties of the insulating film and its interface with the semiconductor. The most important properties revealed by this method are the density of fixed charge in the dielectric film and the energy density of deep levels at the dielectric-semiconductor interface. In some MIS structures, it has been shown that the maximum capacitance (C_{max}) in the accumulation regime increases with decreasing test frequency. Because of this C_{max} increase, the dielectric constant of the AlN film in an AlN/Si MIS structure increases from $5.01\varepsilon_0$ at 1 MHz to $8.65\varepsilon_0$ at 50 Hz [7]. Such behavior is a manifestation of the contribution of deep levels to the polarization properties of the dielectric film. Investigation of the AlN/Si MIS admittance at test frequencies higher than 1 MHz will reveal more clearly the deep level contribution to the change in the dielectric constant of the dielectric film. Such investigations are indispensable for both a comprehensive characterization of the dielectric film properties and the potential use of AlN as high - k dielectric.

The aim of this work is to establish the role of deep levels in MIS structures with PLD AlN films, by studying the admittance of the AlN/Si structure at test frequencies higher than 1MHz.

2. Experimental details

AlN films were prepared by pulsed laser deposition onto p-type (100)Si substrates. During deposition, the substrates were heated to 800°C, the temperature at which

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♣ Paper presented at the International School on Condensed Matter Physics, Varna, Bulgaria, September 2008 the native SiO_2 covering the wafers is known to decompose. This temperature is also high enough to promote the crystalline growth of AlN layers [8]. The target of polycrystalline AlN (99%) was rotated at 0.3 Hz during deposition, 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 ambient nitrogen pressure during the AlN deposition was kept at 0.1 Pa and 10 Pa. The deposited film thickness was measured with an ellipsometer, and was in the range 560 to 760 nm.

Metal-AlN-silicon capacitors were formed by vacuum thermal evaporation through a metal mask of Al dots with an area of 1.96×10^{-3} cm^{-2} on the AlN surface. A continuous Al film was evaporated on the Si backside. The impedance of the formed AlN/Si MIS structures was obtained as a function of applied bias voltage in the 1 – 20 MHz test frequency range, by a measurement setup based on Tesla impedance meter BM 508. The impedance meter simultaneously measured the impedance amplitude $|Z|$ and the phase angle φ. The capacitance, $C_m(V)$, and parallel conductance, $g_m(V)$, values of the investigated AlN/Si structure were calculated from the measured impedance values by

$$g_m(V) = \frac{\cos(\varphi_m(V))}{|Z_m(V)|} \quad \text{and} \quad C_m(V) = \frac{-\sin(\varphi_m(V))}{\omega|Z_m(V)|} \qquad (1)$$

3. Results and discussion

The capacitance-voltage (C-V) characteristics of a MIS structure with an AlN film, deposited at an ambient nitrogen pressure of 10 Pa and measured at test frequencies ranging from 1.08 to 19.05 MHz, are given in Fig.1. At frequencies higher than 14 MHz, the accumulation capacitance appears smaller than the capacitance measured in the inversion condition. Moreover, the reactive (capacitance) component of the current through this AlN/Si structure increases with increasing the frequency. This means that the absolute value of φ_m increases with the frequency, as observed in these impedance measurements. Simultaneously, the impedance amplitude, $|Z_m|$ under accumulation decreases from 1000 Ω at 1.08 MHz to 45–50 Ω at 19.05 MHz. In these ranges of the impedance amplitude, we cannot neglect the influence of the series resistance of the Si bulk and the Al/Si back contact, R_s. At such high frequencies, the R_s value in MIS or MOS structures can be determined from the measured admittance of the structures in the accumulation condition, by the relation [9]

$$R_s = \frac{g_{ma}}{g_{ma}^2 + \omega^2 C_{ma}^2} \qquad \text{or} \qquad R_s = |Z_m|\cos\varphi_m . \qquad (2)$$

Eq. (2) is correct for φ_m values close to $\pi/2$. The series resistance R_s of the investigated AlN/Si MIS structure, estimated in this way, is 26.4 Ω. The obtained value of R_s is independent of the test frequency.

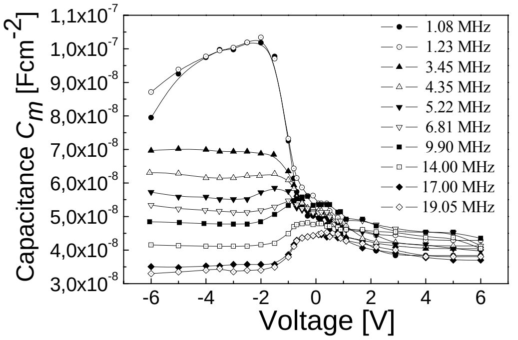

Fig. 1. Measured capacitance C_m as a function of applied voltage for an AlN/Si structure with an AlN film, deposited at 10 Pa nitrogen pressure.

By equating the measured impedance $|Z_m|(\cos\varphi_m + j\sin\varphi_m)$ with the $R_s + \frac{1}{g_d + j\omega C_d}$, we may obtain the real parallel conductance, g_d, and the real capacitance, C_d, of the AlN/Si MIS structure. Then

$$C_d = C_m \frac{\sin^2\varphi_d}{\sin^2\varphi_m} \quad \text{and} \quad g_d = g_m \frac{\cos^2\varphi_d}{\cos^2\varphi_m - R_s g_m} \quad , \quad (3)$$

where $\operatorname{cotg}\varphi_d = \operatorname{cotg}\varphi_m - \frac{R_s g_m}{\sin\varphi_m \cos\varphi_m}$. The corrected capacitances of this AlN/Si structure are given in Fig. 2. Making corrections using Eq. 3, at all frequencies the corrected accumulation capacitances are higher than the inversion capacitances. In our case, the accumulation capacitance, 9.31×10^{-8} Fcm^{-2} at 1.23 MHz, decreases with increasing test frequency and reaches 4.21×10^{-8} Fcm^{-2} at 19.05 MHz. This result demonstrates that deep levels with response time constants between 5.25×10^{-8} s and 8.13×10^{-7} s contribute to the excess capacitance measured at 1.23 MHz, in comparison with the capacitance measured at 19.05 MHz. The sheet energy density of these deep levels, estimated from the excess capacitance, is 3.18×10^{11} $cm^{-2}eV^{-1}$. Assuming a uniform distribution of these deep levels across the AlN film volume, and taking into account the film thickness (560 nm)., one may estimate their volume energy density as 5.68×10^{15} $cm^{-3}eV^{-1}$. The defect concentration in these AlN films is estimated in the 10^{18} - 10^{19} cm^{-3} range from the observed tunneling type DC conduction in them [10]. The observed decrease in the capacitance values can be considered as a decrease in the AlN dielectric constant from $58.88\varepsilon_0$ at 1.23 MHz to $26.63\varepsilon_0$ at 19.05 MHz.

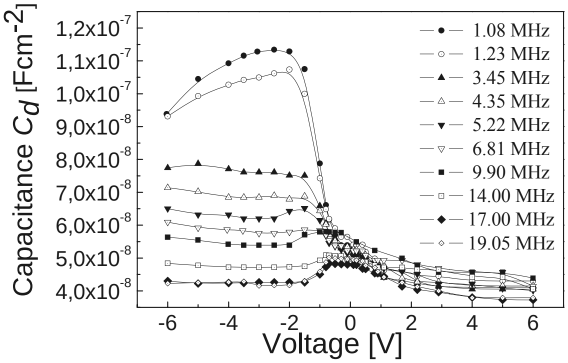

Fig. 2. Corrected capacitance C_d as a function of applied voltage for an AlN/Si structure with an AlN film, deposited at 10 Pa nitrogen pressure.

The measured C-V characteristics of an AlN/Si MIS structure with an AlN film, deposited at a low nitrogen pressure of 0.1 Pa, are given in Fig. 3. In this case, at frequencies ranging from 860 kHz to 18.7 MHz, the accumulation capacitance is higher than the inversion capacitance. Obtained in the same way, the series resistance is R_s =23.6 Ω. This R_s value is close to 26.4 Ω. Taking into account the identical Si substrates for both AlN/Si MIS structures, given in Figs. 1 and 2, one may expect this proximity. Nevertheless, the impedance values of the AlN/Si structure prepared at 0.1 Pa (Fig. 3) are several times higher than those of the 10 Pa AlN/Si structure. Because of this, the corrected accumulation capacitance values with the series resistance are slightly higher than the measured ones. The correction is below 1% at 860 kHz and increases to 12 % upon increasing the frequency to 18.7 MHz. The same correction for the AlN/Si structure, prepared at 10 Pa, is 7% at 1.23 MHz and reaches 28% at 19.05 MHz. In the case of the AlN/Si structure with the 0.1 Pa AlN film, the calculated corrections for the series resistance at all frequencies are smaller than the measurement errors and they are not be taken into account.

The accumulation capacitance of the 0.1 Pa AlN/Si structure measured at 860 kHz is 3.35×10^{-8} Fcm^{-2}, while the same capacitance measured at 18.7 MHz is 3.07×10^{-8} Fcm^{-2}. This result means that deep levels with response time constants between 5.35×10^{-8} s and 8.2×10^{-7} s contribute to the excess capacitance measured at 860 kHz, in comparison with the capacitance measured at 18.7 MHz. The sheet energy density of these deep levels, estimated from the excess capacitance, is 1.83×10^{10} cm^{-2}eV^{-1}. Taking into account the thickness of 760 nm of this AlN film, and assuming a uniform distribution of the deep levels across the film volume, one may estimate the volume energy density of the deep levels as 2.4×10^{14} cm^{-3}eV^{-1}. These values are more than an order of magnitude higher in the 10 Pa AlN film than in the 0.1 Pa AlN film. It is interesting to note that by analysing the slope of *C–V* plots at 1 MHz, it was established that the interface energy density of traps in the 0.1 Pa AlN/Si structure is below 2×10^{11} cm^{-2}eV^{-1}, while in the 10 Pa AlN/Si structure it is above 6×10^{11} cm^{-2}eV^{-1}. Such a significant difference in the deep level density for AlN/Si structures has not been established so far, by other *C–V* characterization methods. The same measurement results (Fig. 3) reveal that the dielectric constant of the AlN film decreases from $29.52\varepsilon_0$ at 860 kHz to $26.99\varepsilon_0$ at 18.7 MHz.

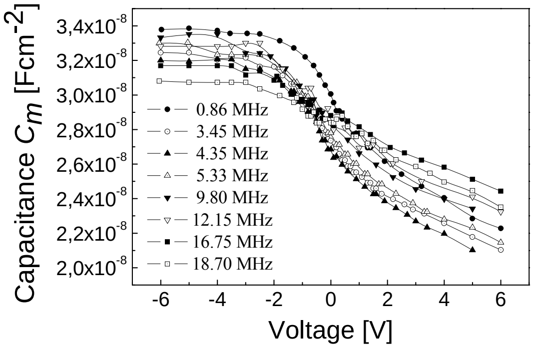

Fig. 3. Measured capacitance C_m as a function of applied voltage for an AlN/Si structure with an AlN film, deposited at 0.1 Pa nitrogen pressure.

In both kinds of AlN/Si structure, the dielectric constant decreases with increasing frequency. The increase of ε_{AlN} with decreasing test voltage frequency is also observed in some other AlN/Si MIS structures, where it is explained with the contribution of nitrogen vacancy dipoles to the value of ε_{AlN} [11]. In [11], it is shown that the AlN dielectric constant in low-pressure MOCVD AlN films decreases from $20.7\varepsilon_0$ to $1.5\varepsilon_0$ when the test voltage frequency increases from 50 Hz to 10 MHz. In our case, the character of the changes in the dielectric constant with the test frequency is the same, but differs quantitatively from those in [11]. Therefore, one may draw the conclusion that the character of the deep levels in PLD AlN films is different from that in MOCVD AlN films. Further investigations are needed to reveal the character of the defects responsible for the obtained admittance characteristics: extended or point defects as in [11].

The corrected parallel conductance of the 10 Pa AlN/Si structure, g_d, at 1.23 and 19.05 MHz, as a function of applied voltage, is given in Fig. 4.

The maximal thickness of the depletion layer, estimated from C-V characteristics measured at 1.05 MHz, is 1.2x10^{-5} cm. Because of the voltage drop across this layer, the conductance under inversion and depletion is smaller than under accumulation. At both measured test frequencies, the maximum current corresponds to the accumulation conditions; the current decreases in the depletion region and increases again in the inversion region. This behavior of g_d is opposite to the change of the capacitance of the AlN/Si structure with changing frequency. Such an a.c. conductance increase with increasing test voltage frequency is observed in many semiconductor and dielectric materials, and is related to charge carrier hopping in the semiconductor or insulator energy gap [12]. In our AlN/Si structure, the current increases by 3–4 times as the test frequency increases by 15–16 times. In contrast to this, in the AlN/Si structure with AlN, deposited at 0.1 Pa nitrogen pressure, g_d is generally smaller than that for the structures with AlN, deposited at 10 Pa. However, when the frequency increases from 860 kHz to 18.7 MHz the current also increases by almost 15 times. This difference in the character of the a.c. conductance increases in both AlN/Si MIS structures needs further investigation.

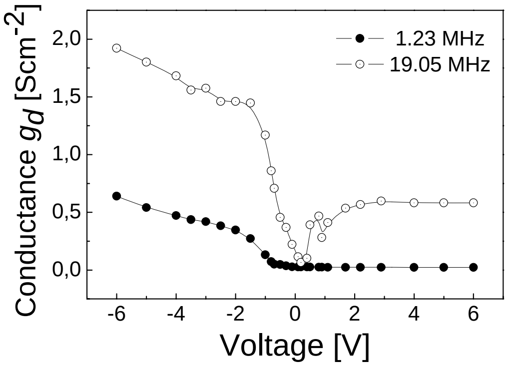

Fig. 4. Corrected conductance at 1.23 MHz and 19.05 MHz as a function of applied voltage for an AlN/Si structure with an AlN film, deposited at 10 Pa nitrogen pressure.

The C-V and G-V characteristics of the 10 Pa AlN-Si structure measured at 77 K and 19.1 MHz differ slightly from the same characteristics measured at 300K. The G-V characteristics are moved by approximately 1 V toward negative voltages, during temperature reduction. From this, it follows that the sheet density of donor-like traps at the AlN/Si interface is $2.3x10^{12}$ cm^{-2}eV^{-1}.

4. Conclusions

It has been established that in the - 20 MHz frequency range, deep levels in pulsed laser deposited AlN films contribute to the AlN/Si MIS structure capacitance under accumulation.

When concentration of deep levels is high enough to obtain correct values for the admittance of the investigated MIS structure, one needs to take into account the series resistance of the semiconductor substrate.

In the 1-20 MHz frequency range, the additional capacitance of AlN/Si structure, connected with deep levels, increases with decreasing frequency. In the same frequency range, under accumulation, the a.c. conductance increases with increasing test frequency.

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