ROMANIAN JOURNAL OF INFORMATION SCIENCE AND TECHNOLOGY
Volume **10**, Number 3, 2007, 251–259

Al/AlN/Si MIS Structures with Pulsed-Laser-Deposited AlN Films as Gate Dielectrics: Electrical Properties

S. SIMEONOV[1], S. BAKALOVA[1], E. KAFEDJIISKA[1], A.SZEKERES[1], S. GRIGORESCU[2], F. SIMA[2], G. SOCOL[2], I. N. MIHAILESCU[2]

[1]Institute of Solid State Physics, Bulgarian Academy of Sciences, Tsarigradsko Chaussee 72, Sofia 1784, Bulgaria
[2]Lasers Department, National Institute for Lasers, Plasma and Radiation Physics, PO Box MG-54, RO-77125, Bucharest-Măgurele, România

Abstract. MIS capacitors with AlN films deposited on p-Si substrates by *pulsed laser deposition* (PLD) have been prepared and the type, energy position and concentration of electrically active defects in the AlN films have been studied. The presence of deep levels has been detected by capacitance-voltage and conductance-voltage measurements performed at different frequencies and temperatures of 77 and 300 K respectively. The concentration of the traps, responsible for the leakage currents, and the conduction mechanism have been determined from the analysis of the current-voltage characteristics at the different temperature regimes. It has been shown that inter-trap tunneling could adequately account for the observed tunneling currents in these MIS structures.

1. Introduction

As the gate silicon oxides of contemporary MOS IC shrink to thicknesses of several nanometers, indispensable quantum-mechanical currents across the gate oxide film severely hinder the IC functioning. Materials with high dielectric constants have been considered as potential substitutes for silicon oxide. Compared with low-permittivity gate dielectrics, more charge is induced for the same applied gate voltage. Accordingly, they can thus be thicker, which would reduce tunneling currents. Bulk AlN has a dielectric constant of $10\varepsilon_0$ compared to $3.9\varepsilon_0$ for SiO_2 [1]. Besides, Aluminum nitride (AlN) is one of the blue and UV light emitting nitrides, which gives it an edge

over other high-k dielectrics. Preparing AlN-Si *metal-insulator-semiconductor* (MIS) structures with acceptable qualities will thus open the path to co-integration of light emitting nitrides with silicon microelectronics. In addition, it is established that AlN-Si interfaces are thermally stable. Many studies have focused on the various methods to prepare AlN-Si structures, including sputtering [2], MOCVD [3], molecular beam epitaxy [4] and pulsed laser deposition, (PLD) [5]. The electrical properties, mainly fixed dielectric charge of AlN-Si MIS capacitors [6] and AlN-Si MISFET [7] have been investigated; however, the specific resistivity of AlN films in these structures was the only parameter that was estimated. The concentration and nature of AlN film defects play an important role in the electro-physical properties of AlN-Si MIS structures. Also, a good understanding of these properties is essential for establishing optimal conditions for AlN deposition by different methods.

The aim of this paper is to study the defects that are responsible for charge transport in PLD grown AlN films. Our results are derived from the analysis of admittance measurements at different frequencies and current-voltage (I-V) characteristics at different temperatures for metal-insulator-silicon (MIS) capacitors with AlN films.

2. Experimental details

AlN films were prepared by pulsed laser deposition on p-type (100)Si substrates. During deposition, the substrates were heated up to 800°C, the temperature at which the native SiO_2 covering the wafers is known to decompose. This temperature also proved to be high enough to promote the crystalline growth of AlN layers [8, 9]. The target consisting of polycrystalline AlN with 99% purity was rotated with 0.3 Hz during multi-pulse laser irradiation in order to avoid piercing. The target-substrate distance was 4 cm. A shutter was introduced between the target and the substrate once the first 1000 laser pulses had been applied. In this way the impurities and defects still present on the target surface could be removed and collected on the shutter before reaching the substrate. The deposition of one structure was performed by applying 20 000 laser pulses generated by an UV KrF^* pulsed laser source ($\lambda = 248$ nm, $\tau_{FWHM} = 7$ ns) operating at a repetition rate of 2 Hz. The laser energy was set to an average of 85 mJ/pulse. The obtained film thickness was about 600 nm, i.e. suitable for the subsequent optical characterizations. The synthesis was performed in nitrogen ambient with pressures of 0.1, 5 or 10 Pa.

For the electrical measurements, metal-AlN-silicon capacitors were formed by vacuum evaporation through a metal mask of Al dots on the AlN surface and a continuous Al film on the Si wafer backside. The capacitance-voltage (C-V) and conductance-voltage (G-V) measurements were carried out at room temperature or 77 K with test voltage frequencies of 15.9 kHz 159 kHz and 1 MHz by using an impedance meter type BM 507 and an E7 - 12 digital LCR meter. The dielectric charge densities were estimated applying the standard high-frequency approximation method [10] based on the comparison of the measured C-V characteristics with the ideal C-V one calculated for the corresponding capacitor with zero defect densities. The current-voltage (I-V) characteristics were measured at 77 K and at room temperature.

3. Results and discussion

The measured C-V characteristics of the studied Al/AlN/Si structures are typical for a MIS structure. Figure 1 illustrates this assertion, where the C-V characteristics of the MIS structure with a 560 nm thick AlN film deposited at 10 Pa nitrogen pressure are given at different frequencies and temperatures.

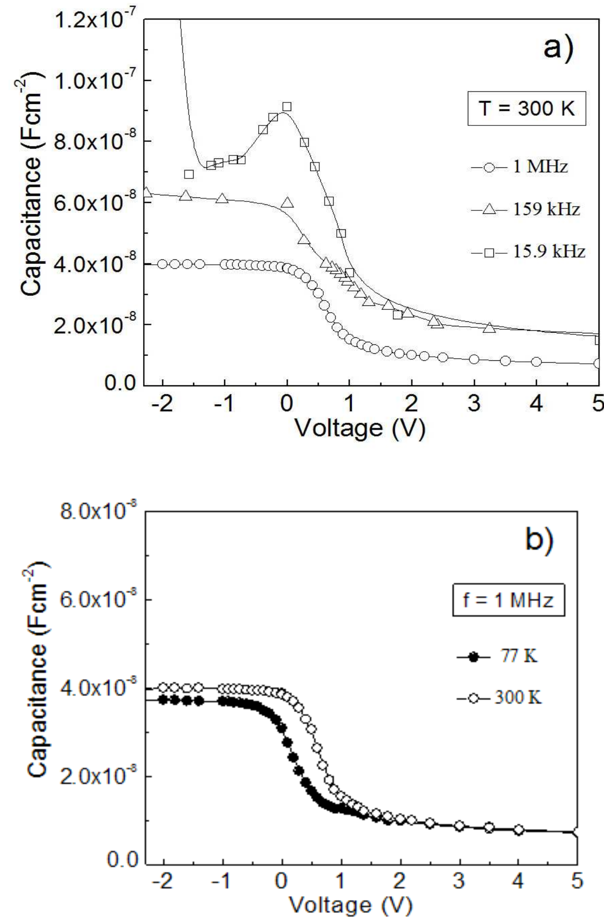

Fig. 1. C-V characteristics of MIS structure with AlN films deposited at nitrogen pressure of 10 Pa in dependence of measurement frequency (a) and temperature (b).

The characteristics measured at 159 kHz and 1 MHz clearly revealed the accumulation, depletion and inversion regions in the C-V plots (see Fig. 1). The 1 MHz C-V plot measured at room temperature was shifted toward more positive voltages compared with the ideal C-V one. This shift has showed that there are fixed dielectric charge built-up in the AlN film with a density of the order of 10^{11} cm^{-2}, which has a

weak tendency to increase with increasing the nitrogen pressure. The related defects were negatively charged, while the fixed oxide charge is always positive in a SiO_2–Si MOS structure.

In Figure 1a one may notice that with decreasing the measurement frequency, the capacitance values become larger in accumulation, depletion and inversion regions. The 15.9 kHz C-V characteristics showed a capacitance maximum in the depletion region, while toward the accumulation region capacitance increased monotonically up to –4 V. The increase by almost one order of magnitude compared with the corresponding capacitance measured at 1 MHz in the depletion region evidence for the presence of interface traps at the AlN-Si interface and of deep levels in Si. The capacitance increase in the accumulation region signals the presence of deep levels in the bulk of AlN film, which capture and emit charge carriers during the voltage sweeps.

As illustrated in Fig. 1b, the 1 MHz C-V characteristics measured at 77 K were shifted toward negative voltages relative to those measured at room temperature. This is an indication of the presence of positively charged traps at the AlN-Si interface, which contributes to the capacitance values moving the Fermi level toward the Si valence band edge during the temperature decrease from 300 to 77 K. Therefore, the AlN-Si interface traps below the middle of the Si energy gap are donor-like. They are of the same nature as the SiO_2 – Si interface traps which are also donor-like in the same part of the Si energy gap [11].

The stretch of the C-V curves along the voltage axis was small revealing low amount of defects related to interface traps (Fig. 1). The concentration of the interface traps was determined from the room temperature 1 MHz C-V curves with the standard high frequency approximation method [10], as the energy distribution of the interface traps density in the Si bandgap is shown in Fig. 2. The considerably flat curves and low densities (below 10^{12} $eV^{-1}cm^{-2}$) over a wide energy region are evident for a good quality interface with an excellent matching of the AlN structure to the Si substrate. The interface traps densities observed for a Si/SiO_2 interface before any thermal treatments are typically higher than 10^{12} $eV^{-1}cm^{-2}$ [12, 13], which is demonstrative of the advantage of the PLD grown AlN on Si.

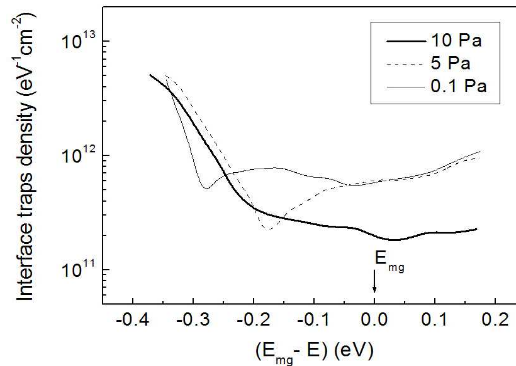

Fig. 2. Interface trap density (D_{it}) distribution in Si bandgap for AlN/Si structures synthesized at different N_2 pressures.

In the case when the concentration of the electrically active defects in the dielectric film is high, the maximum capacitance value differs from the real film capacitance. The contribution of the charge in these bulk traps can be eliminated applying the two-frequency method, as the real film capacitance value C_i can be obtained from the equation:

$$C_i = \frac{f_1 C_1(1 + D_1^2) - f_2 C_2(1 + D_2^2)}{f_1^2 - f_2^2}, \tag{1}$$

where D_1, D_2 is the dissipation ($D = G/|wC|$) and C_1, C_2 the capacitance at two different frequencies f_1 and f_2, respectively. The strong frequency dependence of the C_i in accumulation regime points out the presence of large amount of electrically active defects in our AlN films. Therefore, we calculated the real C_i values from the Eq. (1). The results are summarized in Table 1. The comparison of the measured capacitance values with the calculated ones showed that the 1 MHz C values are close to the real C_i, which suggests that the electron emitting - capturing process cannot follow the ac signal.

Table 1. The measured capacitance of the MIS capacitors in accumulation and the calculated capacitance values of the AlN films without contribution of bulk traps charge

C_i values obtained:	Frequency	Capacitance (Fcm^{-2}) for different N_2 pressures		
		0.1 Pa	5 Pa	10 Pa
Experimentally	1 MHz	2.5	2.4	3.87
Experimentally	159 kHz	3.23	4.08	6.11
Calculation	f_1= 1 MHz, f_2= 159 kHz	2.78	2.68	3.95

The electrically active defects in the AlN films contribute also to the conduction in the MIS structure, as it can be seen from the G-V measurement results. Typical G-V characteristics of an MIS structure are given in Fig. 3 for AlN deposited at nitrogen pressure of 0.1 Pa. The G-V characteristics measured at 1 MHz at room temperature were higher than those measured at 15.9 and 159 kHz in the conditions of accumulation, depletion and inversion (Fig. 3a). These changes in the G-V plots were related to deep levels being present in the bulk of the AlN film and traps at the AlN-Si interface. The 1 MHz G-V characteristics measured at 77 K at accumulation mode were higher than those measured at room temperature (Fig. 3b). This pointed to the presence of deep levels in the AlN film bulk, being responsible for tunneling type conduction in these MIS structures.

The I-V characteristics of the MIS structures were measured in accumulation mode, where the whole voltage drops across the AlN film. Figure 4 shows the I-V characteristics measured at 77 and 300 K for a MIS structure with AlN film deposited at 0.1 Pa and 10 Pa nitrogen pressures.

The specific resistivities, ρ, of the AlN films evaluated from the linear part of the I-V curves in the voltage range from –9 V to –6 V, are given in Table 2. The smallest ρ value is noticed for the highest nitrogen pressure.

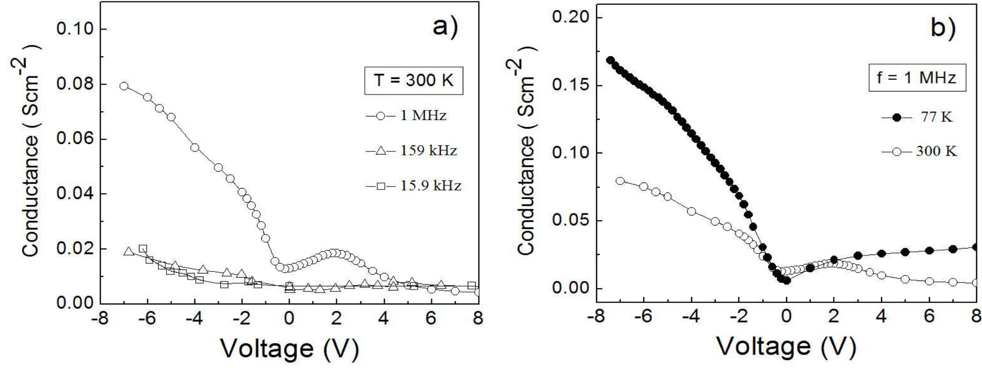

Fig. 3. G-V characteristics of MIS structure with AlN films deposited at nitrogen pressure of 0.1 Pa in dependence of measurement frequency (a) and temperature (b).

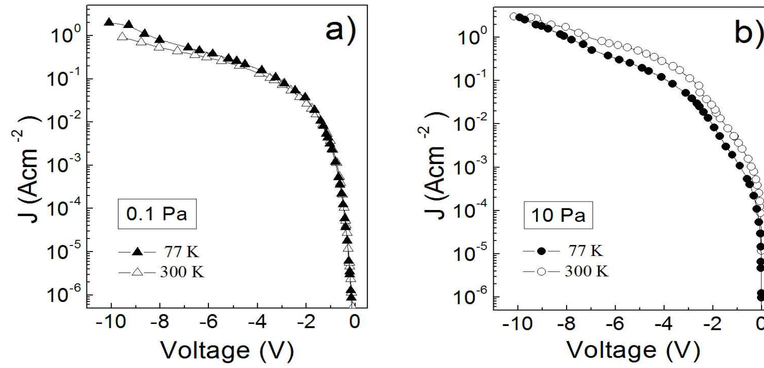

Fig. 4. Typical I-V characteristics, measured at 77 or 300 K, of MIS structure with AlN films deposited at nitrogen with pressure of 0.1 Pa (a) ans 10 Pa (b).

The I-V characteristics in accumulation mode reveal that the current densities have a weak dependence on the temperature. This is an unambiguous proof that the conduction mechanism through the AlN film is of tunneling type. As it has been shown [14], incorporation of Si in AlN transforms AlN into n-type. One may expect that during AlN PLD on Si substrate the film-substrate interaction will turn the AlN film into n-type. If so, then the charge carriers in AlN are assumed to be electrons. The estimated electron effective mass in AlN is in the range of (0.23–0.36)m_e [15]. If one assumes that electrons from occupied deep levels in AlN energy gap tunnel to the AlN conduction band (Fowler-Nordheim emission), the I-V characteristics should be given by:

$$J = J_0 \exp\left[-\frac{4(2m*q)^{1/2}\varphi_t^{3/2}}{3\hbar E}\right], \tag{2}$$

where $q\varphi_t$ is trap energy position in AlN band gap. Using Eq. (2), the energy position $q\varphi_t$ of 23 meV has been calculated from the I-V characteristics in Fig. 3. Such low

values of $q\varphi_t$ are incompatible with the clear dielectric character of investigated AlN films and, therefore, the observed tunneling type currents are not connected with Fowler-Nordheim emission of electrons from the traps in AlN films.

Another conduction mechanism of tunneling type may occur in dielectrics [16]. It is the so-called inter-trap tunneling, where electrons tunnel from occupied deep levels to next-nearest empty deep levels. In this case the I-V characteristics is given by:

$$J = q\nu \frac{1}{w^2} \exp\left[-\frac{2(2m*q)^{1/2}\varphi_t^{1/2} w}{\hbar} \right] \sinh\left[\frac{(2m*q)^{1/2} w^2 E}{\hbar \varphi_t^{1/2}} \right] \qquad (3)$$

Using Eq. (3) and by plotting $\ln J$ as a function of electrical field E in the film, we calculated (Table 2) from the slope of this plot and its intersection with the current density axis, the mean distance w between nearest deep levels and the energy position $q\varphi_t$ of deep levels responsible for inter-trap tunneling. The obtained values of the energy position $q\varphi_t$ = 0.15–0.25 eV are between the values of 0.29 eV of Si donor level [14], and 0.1 and 0.35–0.42 eV reported in [17]. These results show that inter-trap tunneling can explain the observed tunneling type conduction in these AlN–Si MIS structures.

Table 2. The energy position, $q\varphi_t$, and distance, w, of traps in AlN-(p)Si MIS structures

N_2 pressure [Pa]	T_m [°C]	$q\varphi_t$ [eV]	w [10^{-7}cm]	N_t [cm^{-3}]	ρ [Ωcm]
0.1	77	0.2	7.63	2.25×10^{18}	10^5
	300	0.24	6.91	3.03×10^{18}	
5	77	0.15	12.13	5.59×10^{17}	1.5×10^5
	300	0.21	8.29	1.75×10^{18}	
10	77	0.21	7.7	2.18×10^{18}	10^4
	300	0.25	6.66	3.38×10^{19}	

Introducing the w values in the expression $N_t = 1/w^3$, the density of traps responsible for inter-trap tunneling was evaluated. The obtained values of N_t, which are also given in Table 2, were in the range of $5.6\times10^{17} - 3.4\times10^{18}$ cm^{-3}. The low traps density in these AlN films suggests a more ordered and less defective structure leading to higher specific resistivity in comparison with the reported data for AlN films obtained by other techniques [18].

4. Conclusions

The C-V and G-V measurements at different frequencies and temperatures of PLD grown AlN-(p)Si MIS structures manifest the presence of donor-like traps at the AlN-Si interface and deep levels in the AlN film volume. The relatively small densities of fixed charge (of the order of 10^{11} cm^{-2}) and interface traps (below 10^{12} $\mathrm{eV}^{-1}\mathrm{cm}^{-2}$) indicate that AlN-Si interface has a good quality, which makes PLD AlN films potential candidate for gate dielectric for further development in the semiconductor technology.

The lack of dependence of the forward current on temperature indicated tunneling type conduction in AlN films, where the electron tunneling takes place via inter-trap tunneling. The concentration of these traps was in the order of 10^{18}cm^{-3}, a value that correlates well with the specific resistivity of AlN films.

Acknowledgements. The authors acknowledge the support of this work under the Collaboration Agreement between the Bulgarian Academy of Sciences and the Romanian Academy. Theme: "Optical, magnetic and electrical properties of nanostructured layers obtained by PLD for new applications in sensing, waveguides, spintronics, and advanced electrical measurements", 2004–2007.

References

[1] DUBOIS M.A., MULART P., *Properties of aluminum nitride thin films for piezoelectric transducers and microwave filter applications*, Appl. Phys. Lett., **74**(20), pp. 3032–3035, 1999.

[2] FATHIMULLA A., LAKKANI A. A., *Reactively RF magnetron sputtered AlN films as gate dielectric*, Journal of Applied Physics, **54**, pp. 4586–4589, 1983.

[3] ZETTERLING C.-M., OESTLING M., HARRIS C. I., NORDELL N., WONGCHOTIGUL K., SPENCER M. G., *Comparison of* SiO_2 *and* AlN *as gate dielectric for* SiC *MOS structures*, Materials Science Forum, **264–268** , pt. 2, pp. 877–880, 1998.

[4] FAN Z. V., RONG G., NEWMAN N., SMITH J., *Defect annihilation in aluminium nitride thin films by ultra high temperature processing*, Appl. Phys. Lett., **76**(14), pp. 1839–1842, 2000.

[5] LU Y.E., REN Z.M., CHONG T.C., CHEONG B. A., SHOW S. K., WANG J. P., *Ion-assisted pulsed laser deposition of aluminium nitride thin films*, J. Appl. Phys., **87**(3), pp. 1540, 2000.

[6] ADAM T., KOLODZEY J., SWANN C. P., TSAO M. W., RABOLT J. F., *The electrical properties of MIS capacitors with* AlN *gate dielectrics*, Appl. Surf. Science, **175–176**, pp. 428–435, 2001.

[7] Stevens K. S., Kinnibourgh M., Schvartzman A. F., Ohtani A., Beresford R., *Demonstration of a silicon field-effect transistor using* AlN *as the gate dielectric*, Appl. Phys. Lett., **66**(23), pp. 3179–3181, 1995.

[8] VISPUTE R. D., NARAYAN J., WU H., JAGANNADHAM K., *Epitaxial growth of* AlN *thin films on silicon (111) substrates by pulsed laser deposition*, J. Appl. Phys., **77**(9), pp. 4724–4728, 1995.

[9] LIN W. T., MENG L. C., CHEN G. J., LIU H. S., *Epitaxial growth of cubic* AlN *films on (100) and (111) silicon by pulsed laser ablation*, Appl. Phys. Lett., **66**(16), pp. 2066–2068, 1995.

[10] SZE S. M., *Physics of Semiconductor Devices*, Wiley-Interscience, New York, 1969.

[11] LENAHAN P. M., DRESSENDORFER P. V., *Hole traps and trivalent silicon centers in metal/oxide/silicon devices*, J. Appl. Phys., **55**(10), pp. 3495–3499, 1984.

[12] CHENG Y. C., Prog. Surf. Sci. 1977, **8**, 181.

[13] ALEXANDROVA S., SZEKERES A., Phys. Stat. Sol. (a), **92**, 589, 1985.

[14] KANECHIKA M., KACHI T., *N-type* AlN *layer by* Si *ion implantation*, Appl. Phys. Lett., **88**, p. 202106, 2006.

[15] SILVEIRA E., FREITAS JR. J. A., GLEMBOCKI O. J., SLACK G. A., SCHOWALTER L. J., *Excitonic structure of bulk* AlN *from optical reflectivity and cathodoluminescence measurements*, Phys. Rev. B, **71**(4), pp. 202106-7, 2005.

[16] SIMEONOV S., YOURUKOV I., KAFEDJIISKA E., SZEKERES A., *Inter–trap tunneling in thin* SiO_2 *films*, Phys. stat sol .(a), **201**(13), pp. 2966–2979, 2004.

[17] LIGATCHEV V., RUSLI, ZH. PAN, *Density of defect states of aluminum nitride grown on silicon and silicon carbide substrates at room temperature*, Appl. Phys. Lett., **87**(24), pp. 2903–2905, 2005.

[18] RUTZ R. F., *Ultraviolet electroluminescence in* AlN, Appl. Phys. Lett., **28**, pp. 379–381, 1976.