Chapter - 6

METAL-INSULATOR-SEMICONDUCTOR INTERFACE: METAL/HIGH-K/*n*-GaSb MOSCAP

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6.1 Introduction

Device performances have been improved many folds by efforts in scaling down the size of individual transistor elements, but the technology for scaling downof silicon-based CMOS has almost reached its physical limits set by quantum tunnelling through insulation layers and Heisenberg's uncertainty principle that limits the sharpness of etching at a size of 15nm[123-127]. Thus, for higher speeds and lower power operations, it is imperative to develop different materials with whichICs can be made. In this regard, a large number of compound semiconductors are being considered. Among these the most attractive materials appear to be antimony-based III-V compound semiconductors [6-14, 101 & 127]. Although significant work has been carried out on the electron mobility of these materials, hardly any work has been done on hole mobility. But recently, reports of high hole mobility (~ 850 $cm^2V^{-1}s^{-1}$) in GaSb has attracted the attention of many researchers [6-14,125,128-131]. Thus, this material has been chosen for study as a substrate that may provide ICs with greater speeds than that of silicon-based ICsof same size.

Unfortunately, the surface of GaSbis highly reactive to oxygen and forms GaO_x and SbO_x when exposed to air. This is a major roadblock in the use of GaSbas a substrate material for ICs [6,128,130,131]. Furthermore, SbO_x being thermally unstable reacts with the GaSb substrate and forms Ga_2O_3 and elemental Sb. Formation of elemental Sb in GaSb leads to large current leakages and high interfacial trap densities (D_{it}) [128-131]. Generally interface states and fixed oxide charges come into the picture due to the breaking-down or rearrangement of chemical bonds between the oxide and the semiconductor after the oxide has been subjected to a high electric field for some time. This raises a concern about reliability due to changes in the threshold voltage and the current conduction in the device. Thus, prolonged use of the device may causethe circuits to fail. Therefore, to ensure device reliability, one has to control the stress build-up at the interface of the MOS. The quality of the interface and verification of reliability by long-term testingare a few of the steps that need to be investigated.

In this study emphasis has been given to the quality of the oxide-semiconductor interface. Since we did not have the infrastructure to fabricate Metal-Oxide-Semiconductor Capacitors(MOSCAPs), the ideal behaviour of oxide-semiconductor interfaces was simulated using theSILVACO TCAD software. For the purpose of this investigation,high-quality thermodynamically-stable insulators with low interface states (high-K) were chosen for passivation over the GaSb surface. However,a major obstacle is the integration of a high-K dielectric with the GaSb substrate [128-134]. Amongst the different high-K dielectrics, Alumina (Al_2O_3) showsthe best interface properties with the GaSb substrate [128-134].

For greater clarity, this chapter has been divided into four sections:

- A detailed theoretical study of interface properties using high frequency capacitance-voltage (C-V) characteristics by the Terman Method.
- Investigation of the interface properties of Au/Al_2O_3/n-GaSbMOSCAP by C-V analyses using TCADsoftware.
- Investigation of the interface properties from the C-V analyses of high-K dielectrics,Alumina (Al_2O_3) and Hafnium Oxide (HfO_2), on aGaSb substrate with a 2nm Indium Arsenide (InAs) layer used as a surface passivation agent at 300K using a TCAD software.

6.2 Interface TrapDensity

The MOSCAP forms an essential part of a Metal Oxide Semiconductor Field Effect Transistor (MOSFET), which is an important element in the area of VLSI design. Therefore, it is preferred to study the semiconductor-insulator interface quality by analysing the Capacitance-Voltage (C-V) characteristics of a MOS or MIS structure as a function of frequency. During fabrication of the device different kinds of defects get introduced at the oxide-semiconductor interface. Charges trapped at the interface, also known as interface state, are one of the defects thatgenerally reside at the oxide/substrate interface. These trapped charges are due to structural imperfections or dangling bonds. Interface traps are a continuum of energy levels and are quantified as the interface trap density (D_{it}) [1-3, 6,127-132,136-138]. These are electrically active defects and are situated within the band-gap, and also exist within the conduction & valence bands, but are indistinguishable from the large density of band states. The D_{it} act as generation/

recombination centres and contribute to current leakage, low frequency noise, reduced mobility, drain current and trans-conductance and is expressed by the formula

$$D_{it} = \frac{C_i}{q}\left[\left(\frac{d\psi_s}{dV}\right)^{-1} - 1\right] - \frac{C_d}{q} \tag{6.1}$$

Where, C_i is insulating capacitance, C_d the depletion capacitance and $\psi_s$is the surface potential.

The high-frequency method was first developed by Terman. The advantage of the high-frequency method is that it does not contain the interface trap associated capacitance C_{it} in the equivalent circuit. The following steps are required in order to calculate the interface trap charge density [2],

Step 1: The energy band diagram has been takenfromthe manual of different gate voltages ofthe simulated MOSCAP structure. From the band bending, the depletion region width (W_{dep}) needs to be determined for each applied gate voltages.

Step 2: From the obtained value of depletion region width, the surface potentials need tobe computed using the formula:

$$\phi s = \frac{q\, N_a W_{dep}^2}{2\varepsilon_s} \tag{6.2}$$

Step 3: The function, F, needs to be calculated using following formula.

$$F\left(\beta\psi_s, n_{po}/p_{po}\right) = \sqrt{\left(e^{-\beta\psi_d} + \beta\psi_d - 1\right) + \left(n_{po}/p_{po}\right)\left(e^{\beta\psi_d} - \beta\psi_d - 1\right)} \tag{6.3}$$

Step 4: The Debay length L_d needs to be calculated:

$$L_d = \frac{\varepsilon_s}{q p_{po} \beta} \tag{6.4}$$

Step 5: The depletion region capacitance $C_d$needs to be calculated using the following formula.

$$C_d = \frac{\varepsilon_s}{\sqrt{2}\times L_d}\left[\frac{1 - e^{-\beta\psi_s}\left(n_{po}/p_{po}\right)\left(e^{\beta\psi_s} - 1\right)}{F\left(\beta\psi_s, n_{po}/p_{po}\right)}\right] \tag{6.5}$$

Step 6: Using the relation between depletion region capacitance, insulating capacitance, the slope of a surface potential (ψs) and from C curve the interface charge density (D_{it}) needs to be calculated:

$$D_{it} = \frac{C_i}{q}\left[\left(\frac{d\psi_s}{dV}\right)^{-1} - 1\right] - \frac{C_d}{q}$$

6.3 Simulation Details

6.3.1 Au/Insulator/n-GaSb MOSCAP

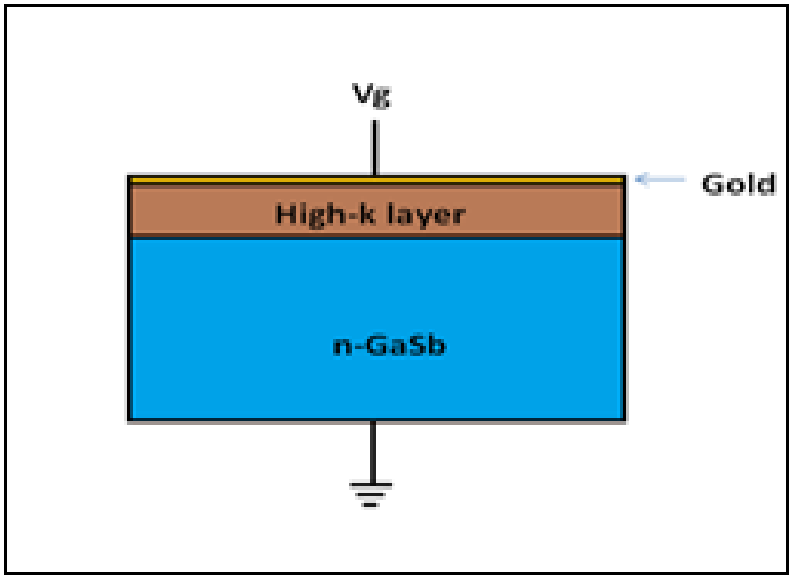


Figure 6.1. Proposed structure of a MOSCAP without substrate passivation

The Atlas TCAD software (version 5.10.0.R)fromSILVACO comprises of several modules to generate the device and finite element methods are used to perform the simulation [69]. Ahigh-K/n-GaSb simulated MOSCAP structure, as shown in Figure 6.1,withadimension of 40nm x 30nmwas chosen. The Tellurium doping profile assigned for GaSb was $5x10^{17}cm^{-3}$ at room temperature. An ohmic contact was placed at the bottom of the substrate usingan Indium (In) contact andgold (Au) as a gate contacthas been fedinto the software. The entire simulated structure was divided into 600 triangles with 341 grid points. A denser mesh near the oxide semiconductor interface (high-K/GaSb interface) was considered for an in-depth investigation of the interface properties. For MOS simulation the parameters Shockley-Read-Hall recombination model (SRH)and Continuously Variable Transmission model (CVT) define the recommended models. Basic for the SRH model are thedrift-diffusion assumption for the transport of electrons and holes, whereas that of CVT model sets a general purpose mobility model that includes concentration, temperature, parallel field and transverse field dependence. The Newton-Gummel iteration method was used for simulation. Newton method solves the total system of unknowns together.

Whereas, Gummel method solves each unknown in turn, keeping the other variables constant and the process repeats till a stable solution is achieved [69].

6.3.2 Au/High-K/InAs/n-GaSb MOSCAP

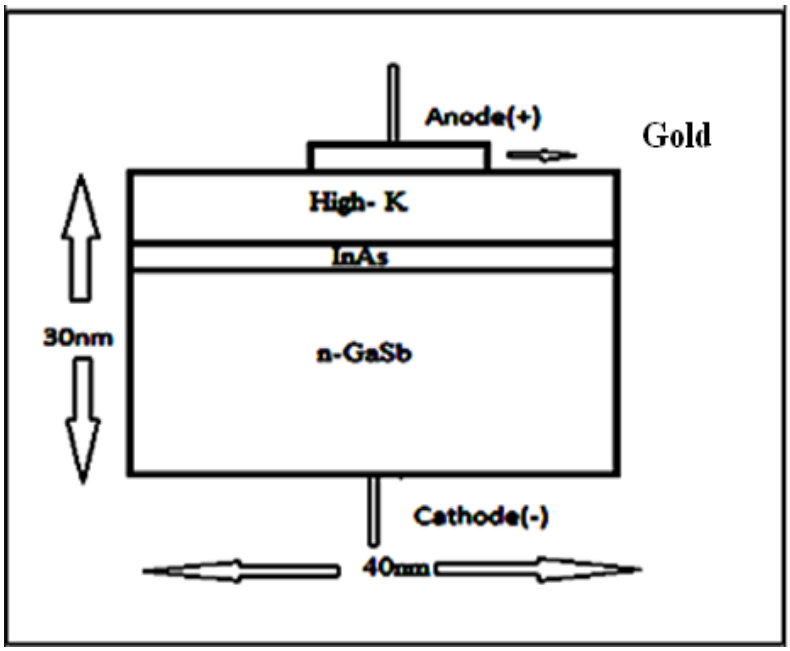


Figure 6.2 Schematic Diagram and Sign Convention of the Proposed MOSCAP Structures with Surface Passivation Layer

A two-dimensional numerical simulation was carried out using the ATLAS TCAD software. A program was developed separately in DECKBUILD window interfaced with ATLAS for calculating different characteristics of the proposed MOSCAP device, as shown in Figure 6.2. A single gate MOS capacitor on an n-GaSb substrate, high-K as gate oxide with InAs as surface passivation layer has been considered with Aluminum as the gate material. Carrier and doping densities were calculated using Fermi-Dirac statistics for the n-type GaSb substrate and Tellurium doping of $5x10^{17}cm^{-3}$was considered,which is same as that of the structure used without passivation in the previous section. Two different high-K oxides like Al_2O_3 and HfO_2 of 5nm thickness were introduced. In between the high-K and n-GaSb substrate, a 2nm thick layer of InAs has been taken as the surface passivation layer. The 2nm thickness of the InAs layerhas calculated from Vegard's law to avoid the strain [139] that may appear due to lattice mismatch between the substrate and the surface passivation layer. Finally at the bottom of the structure, an ohmic contact was placed in contact with thesubstrate. The typical dimensions of a 40nm x 30nm thick device

structure were considered for simulations as shown in Figure 6.2.The entire simulated structure has been divided into 880 triangles with 495 grid points. Just like the structure discussed in the previous section, a denser mesh has been considered at the interface for an in-depth study of the interface properties. Besides this, just like in the previous structure described the Newton-Gummel iteration method and models like SRH and CVT were included for this structure also [69]. Finally capacitance-voltage measurements were simulated by superimposition of a small sinusoidal AC signal on the DC voltage sweep with an appropriate polarity at different frequencies.

6.4 Results and Discussion

At first the Au/ZnO/n-GaSb structure has been simulated using the ATLAS TCAD software. The electrical characteristic of Au/ZnO/n-GaSb MOSCAP has been studied using the Capacitance-Voltage (C-V) characteristics at a frequency of 1 MHz. The D_{it} information, extracted from the C-V characteristics of Au/ZnO/n-GaSb MOSCAP structure using the Termann method, was found to be in the order of 10^{18} cm^{-2} eV^{-1}.A high value of interface trap density was obtained which indicates a low quality of interface between Zinc Oxide and GaSb from the point of view of fabricating MOSCAPs. Therefore, other oxides were considered in place of ZnO for further investigation. Two MOSCAP structures were considered for study, one with high-K on n-GaSb and other one with high-K on n-GaSb substrate with a 2nm InAs layer used as surface passivation. For the high-K's the dielectrics Al_2O_3 and HfO_2 were chosen as insulators at 300K in the TCAD software.

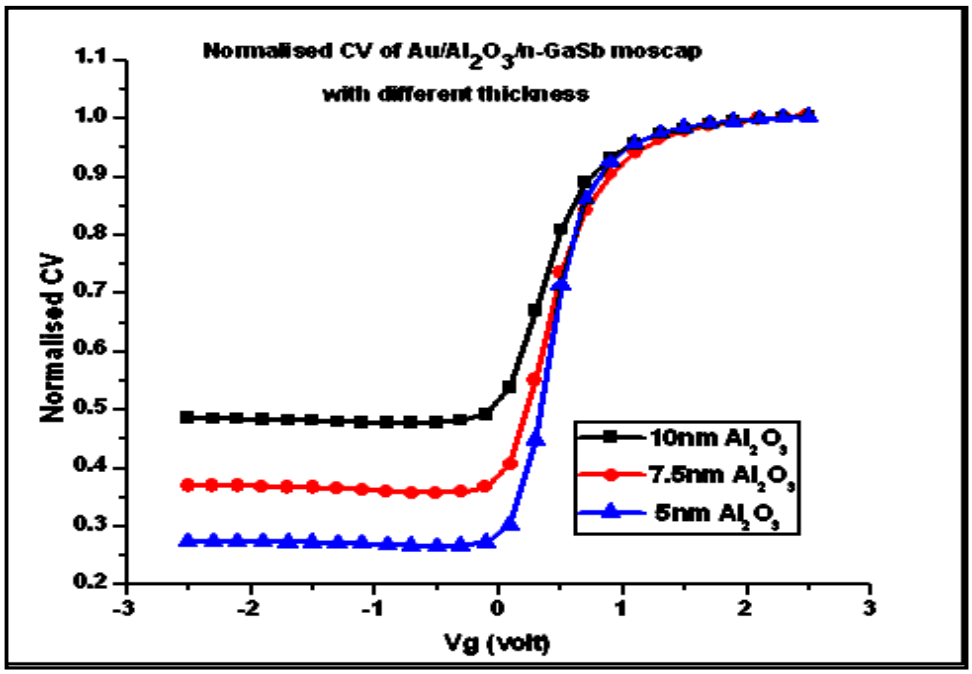


Figure 6.3. Normalised CV Characteristics of Au/Al_2O_3/n-GaSb MOSCAP Structure for Different Thicknesses of Al_2O_3

Figure 6.3 shows the normalised C-V characteristics of the Au/Al_2O_3/n-GaSb MOSCAP simulated using the TCAD softwarefor various thicknesses of Al_2O_3 ranging from 5nm to 10nm. Further analyses havebeen made based on the results determinedfrom the y-parameter output matrix, which contains the conductance and the capacitance information for each electrode of the device. It is evident from Figure 6.5that on normalisation, the CV characteristics of Au/Al_2O_3/n-GaSb MOSCAP structure, the accumulation region capacitance decreases for increasing thickness of Al_2O_3 (5nm, 7.5nm, 10nm) as the oxide capacitance is related to permittivity and thickness of the oxide layer.

The D_{it} information determined from the C-V characteristics of Au/Al_2O_3/n-GaSb MOSCAP structure using the Terman method has been plotted in Figure 6.4. It is evident from the figure that the introduction of Al_2O_3 improves the interfacial property as D_{it} reduces with increasing Al_2O_3 thickness [128-135,138]. The D_{it} value has been found to reduce to 10^{13} cm^{-2} eV^{-1} for the Al_2O_3/n-GaSb interface. A similar trend of decreasing D_{it} had been reported for a Ni/Al_2O_3/p-GaSb MOSCAP structure createdto demonstrate a-Si interface passivation layer [140].

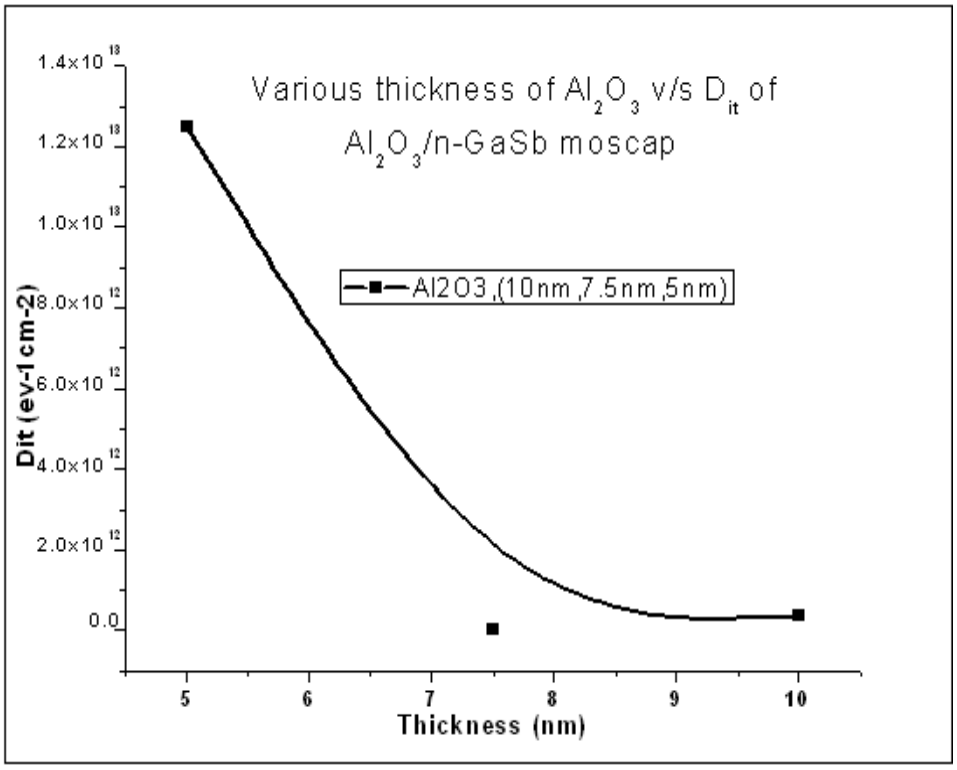
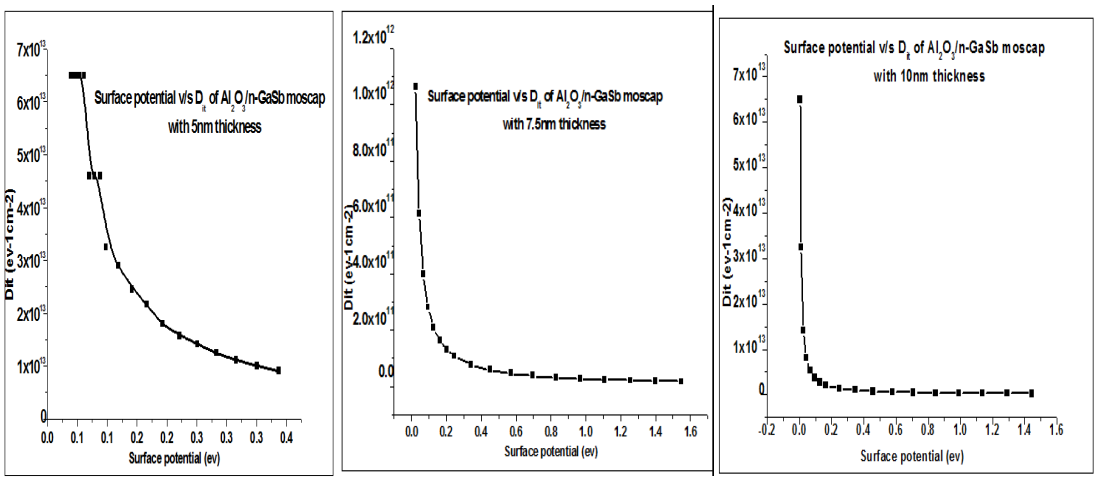


Figure 6.4. Oxide Thickness v/sD_{it} of Au/Al_2O_3/n-GaSb MOSCAP Structure for Different Thicknessesof Al_2O_3

Figures 6.5 (a),(b) and (c) represent the interface trap density distribution as a function of the surface potential ata 1MHz frequency response inAu/Al_2O_3/n-GaSb MOSCAPs for different thicknesses of Al_2O_3. This distribution approximates the interface trap density $D_{it,min}$ at the mid gap at a surface potential,$\Phi_s \approx$ 0.3eV. This is due to the assumption that D_{it} are donors in the upper half and acceptors in the lower half of the band gap, as explained elsewhere[136].



(a) (b) (c)

Figure 6.5. Surface Potential v/sD$_{it}$ of Au/Al$_2$O$_3$/n-GaSb MOSCAP Structures for Different Thicknessesof Al$_2$O$_3$(a) 5nm (b) 7.5nm (c) 10nm

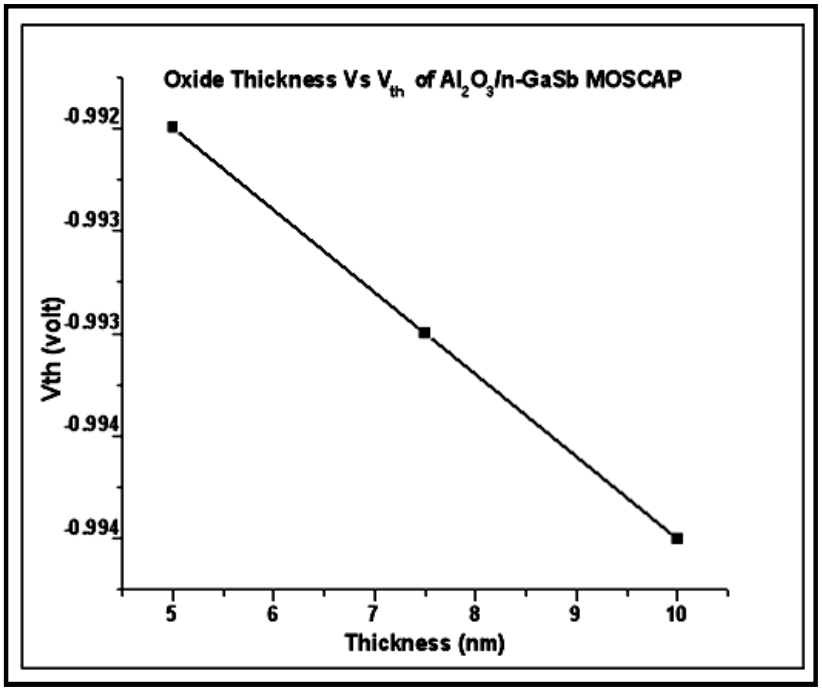


Figure 6.6(a).Oxide Thickness v/sV$_{th}$for Au/Al$_2$O$_3$/n-GaSb MOSCAP

The threshold voltage and flat band voltage were also calculated. It was found from Figure 6.6 (a) & (b) that the device threshold voltage, and so the flat band voltage decreases with the increase of oxide thickness. These effects may be due to varying work function difference, fixed charge density and interface charge density located at the high-k/GaSb interface [2].

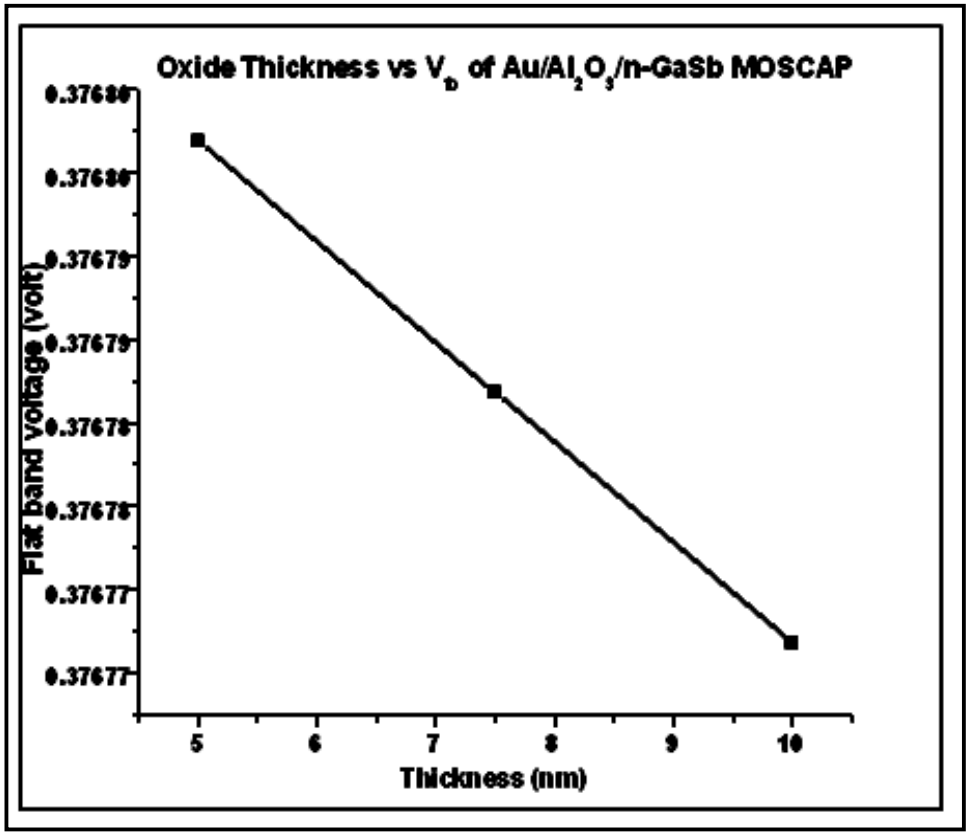


Figure 6.6(b)Oxide Thickness v/sV_{fb} for Au/Al_2O_3/n-GaSb MOSCAP

After the detailed interface analysis of Al_2O_3/n-GaSb MOSCAP without the passivation layer, it was concluded that further improvement of the interface quality was needed. From extensive literature survey it was found that improvement is possible by introducing a surface passivation layer sandwiched between the high-Ks and GaSb surface. Therefore, a systematic study of interface charges (D_{it}), threshold voltages (V_{th}) and flat band conditions (V_{fb}) was done using the Capacitance-Voltage (C-V) technique for different high-Kdielectrics(Al_2O_3 and HfO_2) on n-GaSb substrate with an InAs surface passivation layer at 300K using the TCAD software. To simulate the electrical properties of MOS capacitors appropriate material parameters were chosen from various references, shown in Table 6.1. Prior to carrying out simulation of all three structures, the validation of simulation results of Al_2O_3/InAs/n-GaSb MIS structure was done againstavailable literature [138].

Table 6.1: Summary of Parameter Values Used in the current Simulation at 300K [6,61,91& 95]

Symbol	Description	Value
E_g	Bandgap of GaSb	0.72
K	Permittivity of GaSb	15.7
Ni	Intrinsic carrier concentration of GaSb	$3.54x10^{12}$
V_{sat}	Saturation voltage of GaSb	$1x10^{6}$
E_g	Band gap of InAs	0.35
K	Permittivity of InAs	15.2
N_i	Intrinsic carrier concentration of InAs	$1x10^{15}$
K	Permittivity of Al_2O_3	9
K	Permittivity of HfO_2	13
φ_m	Work function of Au	4.08

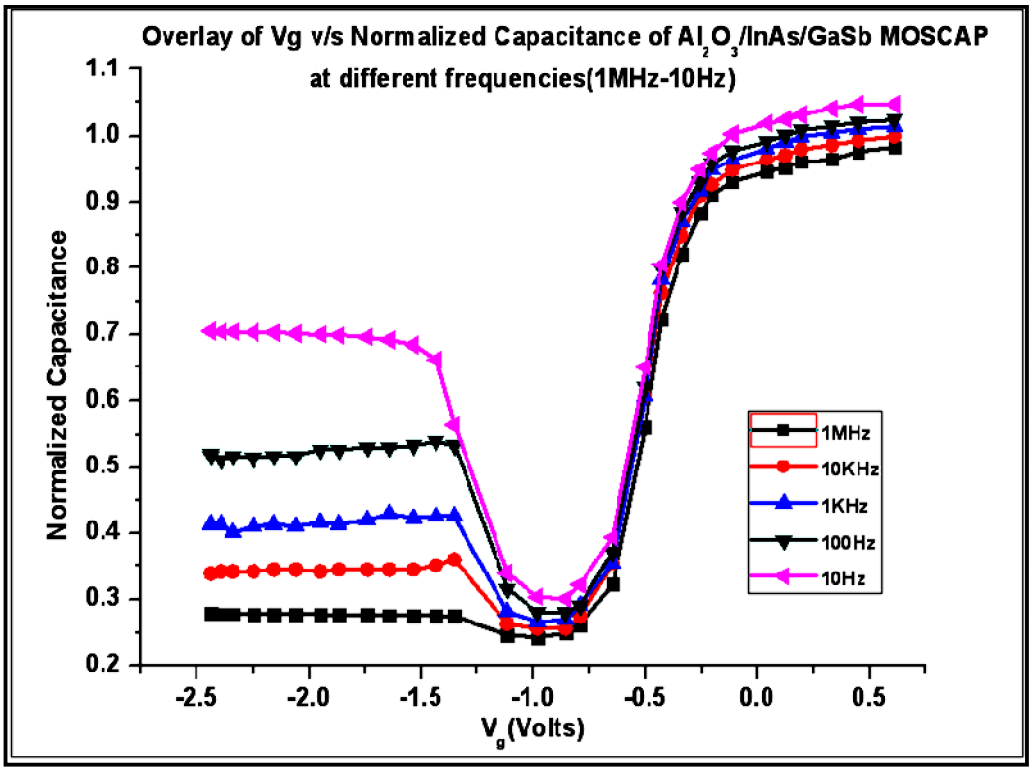


Figure 6.7 Multi-frequency Capacitance-Voltage Characteristics of$Au/Al_2O_3/InAs/n$-GaSb MOSCAPs

The multi frequency capacitance voltage plotted from 10Hz to 1MHz in a simulation is shown in Figure 6.7. It is found that Al_2O_3 shows a better interface property

with an InAs passivated GaSb substrate, shows distinguished accumulation, depletion and inversion region. But a significant amount of frequency dispersions were found at the accumulation region that indicates the presence of interface trap densities (D_{it}).The calculated D_{it} was found to be 3.38 x10^{12} $cm^{-2}eV^{-1}$ which is reasonably close to the experimentally determined value of $D_{it}\approx$ 2-3 x10^{12} $cm^{-2}eV^{-1}$[138].

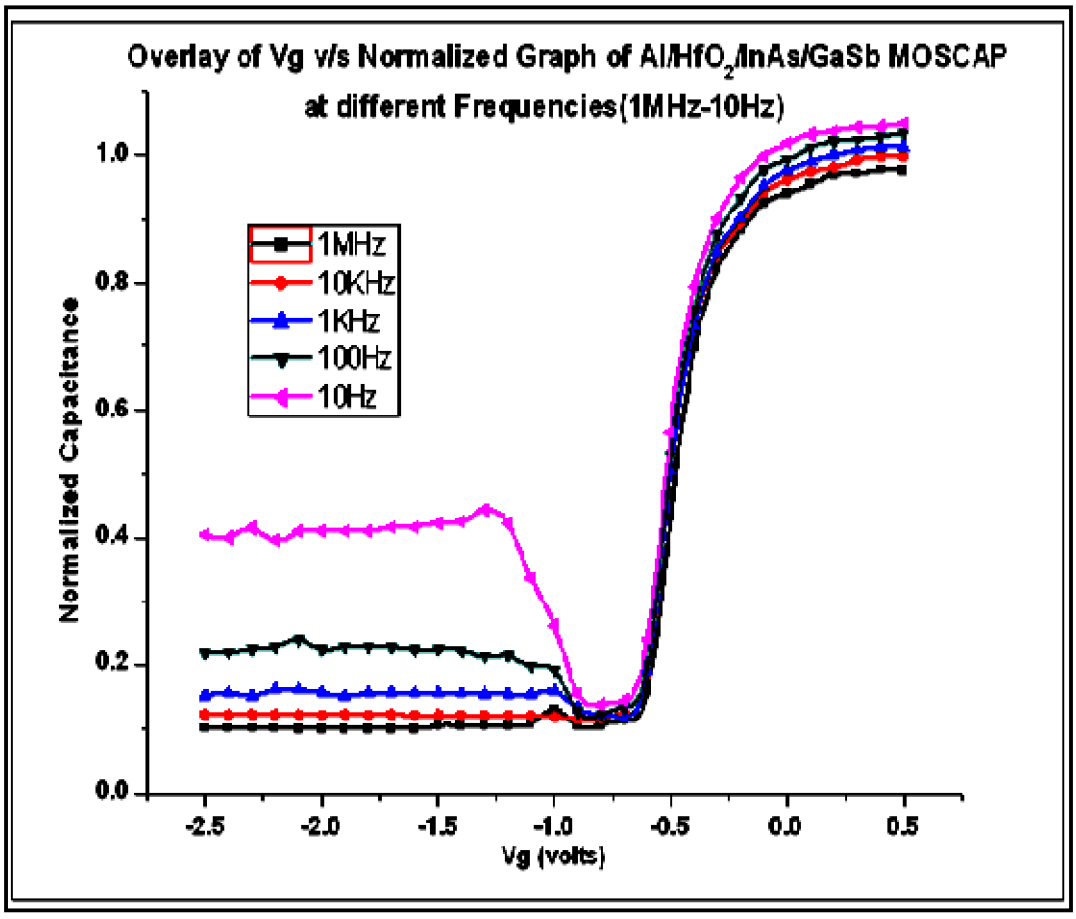


Figure 6.8 Multi-frequency Capacitance-Voltage Characteristics ofAu/HfO_2/InAs/n-GaSb MOSCAP

After verification of the simulated result of Au/Al_2O_3/InAs/n-GaSb MOSCAPs, HfO_2 (~ 25) high-Kwas considered for the next study. Figure 6.8 shows the simulated multi-frequency capacitance voltage plots for the Al/HfO_2/InAs/n-GaSb MOSCAP structure. In HfO_2/InAs/n-GaSb frequency dispersion in the accumulation region is less compared to Al_2O_3/InAs/n-GaSb MOSCAP structure. The fall from the accumulation to depletion is sharper in case of HfO_2/InAs/n-GaSb. This indicates that InAs passivation gives a better interface between HfO_2 and GaSb substrate. Furthermore, with HfO_2/InAs/n-

GaSbthe MOSCAP structure shows less frequency dispersion in the accumulation region indicatingsuppression of border traps near the interface. The smaller frequency dispersion and strong gate dependent modulation can only be possible if the device possesses good quality dielectric and good interface properties.

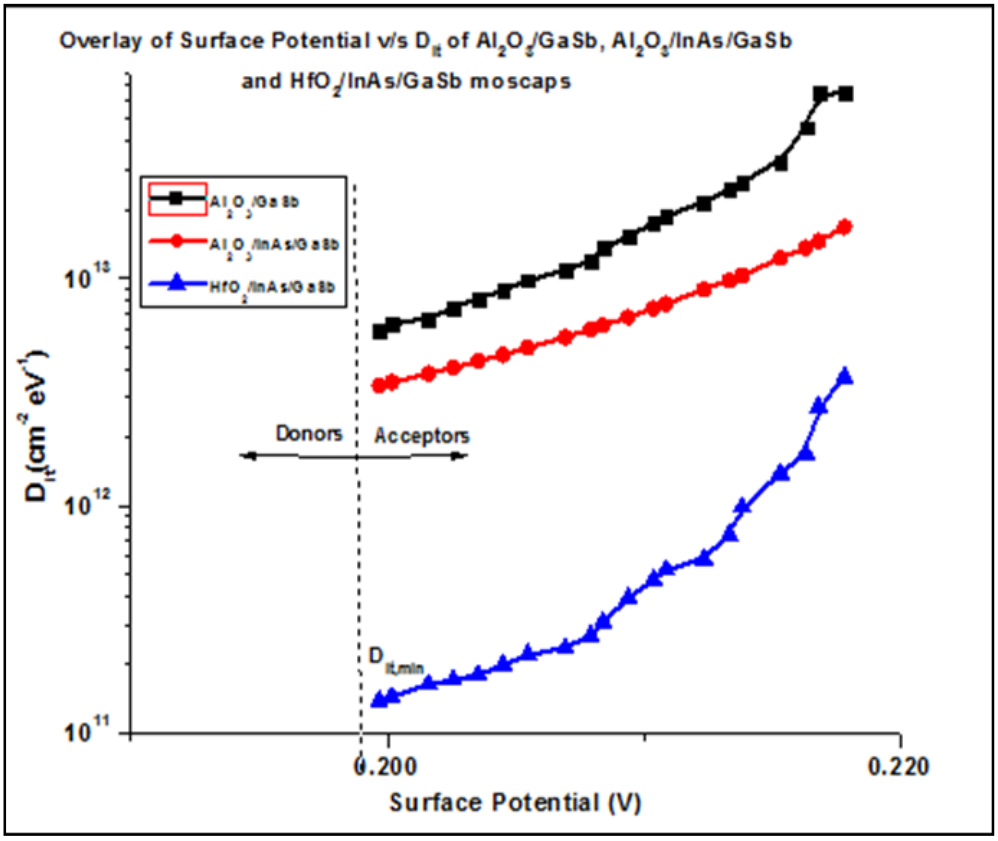


Figure 6.9 Interface Trap Distribution for Al_2O_3/n-GaSb , Al_2O_3/InAs/n-GaSb and HfO_2/InAs/n-GaSb MOSCAP Structures

The interface trap density for all the three MOSCAP structures with InAs passivation has been shown in Figure 6.9 as a function of surface potential. The interface trap density distribution with respect to the surface potential shows the $D_{it,min}$ of the high-K/GaSb interface at the midgap. The discontinuity at $\phi_s \approx 0.2V$ may be due to the fact that D_{it} acts as a donor in the upper half and as an acceptor in the lower half of the band gap. At low density clusters, a few oxide charges are adequate to form the interface trap levels near the band edge. If high density cluster charges exist then an interface trap levels near the midgap would have occurred, but this possibility of this happening is rare [136]. The calculated D_{it}, found to be $1.15x10^{12}$ $cm^{-2}eV^{-1}$ for the HfO_2/InAs/n-GaSb MOSCAP

structure, shows a significant reduction of trap states. When compared with the Al_2O_3/InAs/n-GaSb structure, D_{it} found for the HfO_2/InAs/n-GaSb structure is reduced by 65% .Thus the D_{it} for HfO_2/InAs/n-GaSb MOSCAP gives the lowest value of $1.15x10^{12}$ $cm^{-2}eV^{-1}$as compared tothe other two MOSCAP structures.

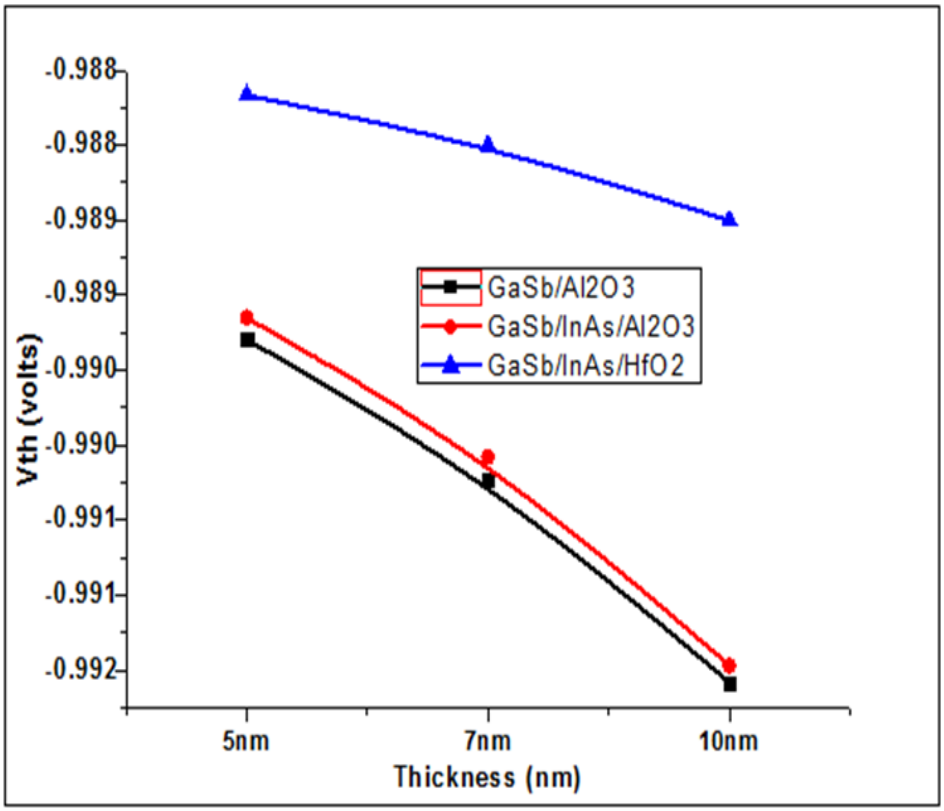


Figure 6.10 Oxide Thickness v/s Threshold Voltage ofAl_2O_3/GaSb,Al_2O_3/InAs/GaSb and HfO_2/InAs/ GaSb MOSCAPS

Besides the interface density (D_{it}), other vital electrical parameters like threshold voltage (V_{th}) and flatband voltage (V_{fb}) were estimated at 300K. In all the proposed structures oxide thicknesses variedfrom 5nm to 10nm. Figure 6.10 shows the variation of the threshold voltage with different oxide thicknesses. For higher oxide layer thickness of Al_2O_3 in Al_2O_3/InAs/GaSb MOSCAP there was adecrease in threshold voltage. On the other hand, higher oxide layer thickness not only reduces the sub-threshold leakage, but also exponentially reduces tunnelling current as reported[141]. From the results of Al_2O_3/InAs/GaSb and HfO_2/InAs/GaSb MOSCAPs it is clear that change in threshold voltage with oxide thickness is almost insignificant. Therefore, the proposed HfO_2-based

structurescan be used for high performance devices,especially in deep submicron p-MOSFETs devices.

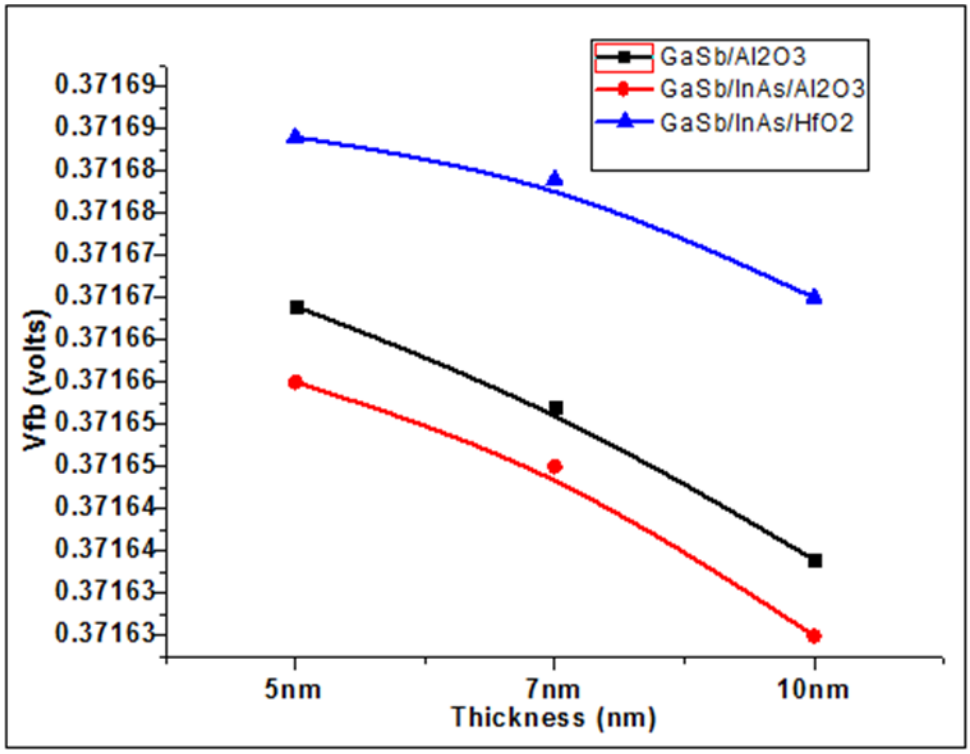


Figure 6.11 Oxide Thickness v/s FlatBandVoltage ofAl_2O_3/GaSb, Al_2O_3/InAs/ GaSb and HfO_2/InAs/ GaSb MOSCAPs

Furthermore, the flatband voltages were derived from the high frequency C-V plots for all the three proposed MOSCAP structures for different oxide thicknesses. Figure 6.11 shows the flatband voltage versus oxide layer thickness showing the effect of varying work function difference, fixed charge density and interface charge density located at the high-K/GaSb interface.

6.5 Chapter Summary

Thefirst part of our study suggests that the GaSb substrate is a useful material for*p*-MOSFETsin attempting to improve device performance without changing the basic structure of the device. The Au/ZnO/*n*-GaSb MOSCAP structure shows a very high value of interface trap densitysuggestinga low quality interface between the ZnO and the GaSb from MOSCAP point of view. On the other hand, a high-KAl_2O_3 layer not only shows better interface properties but also shows good thermally stable insulator propertyfor a

highly reactive substrate like GaSb. Therefore, rigorous simulation neededbe carried out by the use of physical models and device simulation before fabrication of the actual device.

In the second part of the study, interface charge density, threshold voltage and flatband voltage were estimated by C-V characteristics of Al_2O_3/InAs/*n*-GaSb, HfO_2/InAs/*n*-GaSb and compared with Al_2O_3/*n*-GaSb MOSCAPs by a TCAD tool at 300K. In two structures considered,with 5nm thickness of Al_2O_3 and HfO_2 dielectric layers respectively,both with 2nm thicknesses of InAs passivation on GaSb substrate were taken. It is interesting to note that the D_{it} of Al_2O_3/InAs/*n*-GaSb and HfO_2/InAs/*n*-GaSb with respect to Al_2O_3/*n*-GaSb were reduced by 34% and 65% respectively. The threshold voltage (V_{th}) and flatband voltage were found for all the proposed structures with various oxide layer thicknesses ranging from 5nm to 10nm. Furthermore, the lowest threshold voltage and flatband voltage variation with oxide layer thickness were found in the HfO_2/InAs/GaSb structure as compared to the other two structures. Based on this interface study the conclusion may be drawn that HfO_2/InAs/GaSb structure should be a preferredchoice for high performance deep submicron *p*-MOSFETs devices.