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Visualization of Interface Trap Distribution for Pd/AIN/6H-SiC and Pd/HfO₂/6H-SiC MOS Capacitors at 700 K

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Abstract. Comparison of C-V characteristics and interface trap distribution for 6H-SiC MOS capacitor with AlN and HfO₂ as high-k dielectric are presented. It is observed that the transition from accumulation to inversion requires a small change in gate voltage for HfO₂ compared to AlN. Furthermore, larger shift in flat band voltage with respect to frequency is observed in case of AlN. A larger change in capacitance with respect to voltage and flat band voltage shift with respect to frequency for AlN indicated a poor choice for MOS capacitor compared to HfO₂.

Introduction

Apart from silicon carbide (SiC) MOSFET's and Schottky diodes, SiC based metal oxide semiconductor (MOS) capacitors has been implemented for gas sensing applications [1]. The presence of these devices as gas sensors in harsh environment exhaust streams help in minimizing pollution. However, these devices are limited by oxide reliability at high temperature. Due to the presence of high level of interface traps with silicon dioxide (SiO₂), other high-k dielectric layers have been extensively explored [2], [3]. In this study, a comparison in terms of C-V characteristics and trap distribution between the two commonly used high-k dielectrics (AlN and HfO₂) for SiC is reported. The aim is to identify the suitable high-k dielectric for SiC MOS structure used in sensor applications considering same interface trap distribution.

Methodology

The SiC MOS structure shown in Fig. 1 is constructed and simulated using the synopsys sentaurus device simulator at a fixed oxide thickness (50 nm) and lattice temperature (700 K). A fixed oxide charge of 1E12 cm⁻³ is defined in the oxide along with uniform distribution of oxide-interface traps (2E12 cm⁻².eV⁻¹ - 1E13 cm⁻².eV⁻¹) from mid bandgap to conduction band. In the presence of hydrogen (H₂) environment, a decrease in metal work function was reported by the presence of H₂ atoms at the surface [4]. The value of Pd (Palladium) work function has been changed to 4.12 eV (from 5.12 eV), to take the influence of H₂ into account. Palladium is chosen as gate material due to solubility of H₂. The electrical simulation of the device requires accurate mesh resolution at interfaces and field oxide corners which resulted in 25,000 mesh nodes. The physical models include recombination-generation process (R-G) or Shockley-read-hall (SRH) process with doping and temperature dependency, auger recombination model [5]. Mobility along the interface modelled by Philips unified mobility model (Phumob) and Lombardi model to account for the mobility degradation at AlN/SiC and HfO₂/SiC interface due to acoustic phonon scattering, electron-hole scattering and surface roughness. Doping dependence, field dependence, and incomplete ionization, anisotropic effects were considered into effect to predict the performance accurately. The influence of interface traps on C-V characteristics of the MOS capacitor are analyzed at high frequency (1 MHz) by varying the interface trap density from 2E12 cm⁻²eV⁻¹ to 1E13 cm⁻²eV⁻¹. The fixed and uniform trap distribution is analyzed for both AlN/SiC and HfO₂/SiC structures at 700 K with respect to band energy levels. For better analysis frequency is varied (1 kHz – 10 MHz) to observe the flat band voltage (V_{FB}) shift for both structures at 700 K.

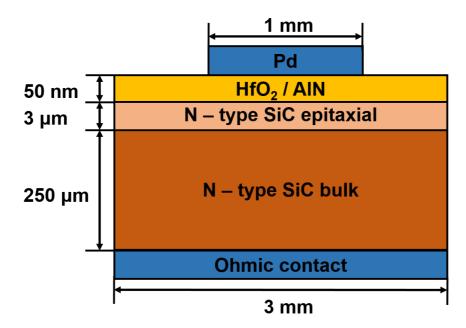


Fig. 1. Schematic cross-sectional view of 6H-SiC MOS capacitor with high-k HfO₂/AlN as dielectric.

Results and Discussion

The sensitivity to hydrocarbons can be related to changes in capacitance at a constant gate voltage. In other words, there should be constant capacitance in accumulation and inversion regions and steep slope in the depletion region. Fig. 2a and Fig. 2b show the maximum capacitance normalized C-V curves between hafnium oxide (HfO₂) and aluminum nitride (AlN) dielectrics at different interface trap densities. Interestingly, there is a decrement in the capacitance value in the accumulation region for AlN-SiC interface which is absent for the HfO₂-SiC interface. This result means that AlN has inferior interface properties compared to HfO₂.

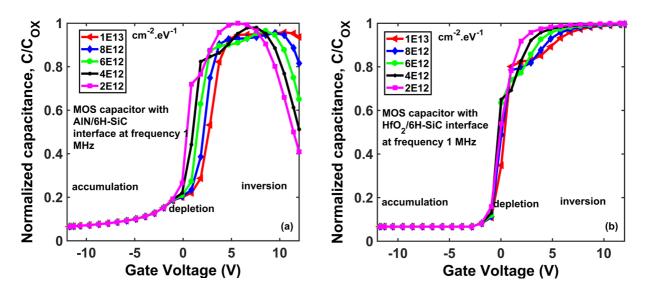


Fig. 2. Normalized C-V characteristics of (a) Pd/AlN/6H-SiC and (b) Pd/HfO₂/6H-SiC capacitor at different trap concentrations.

Fig. 3a and Fig. 3b show the trap density as a function of band gap energy for AlN-SiC and HfO₂-SiC interface respectively. Uniform distribution of traps from mid band gap to the conduction band and an exponential distribution closer to the conduction band edge has been defined at the interface.

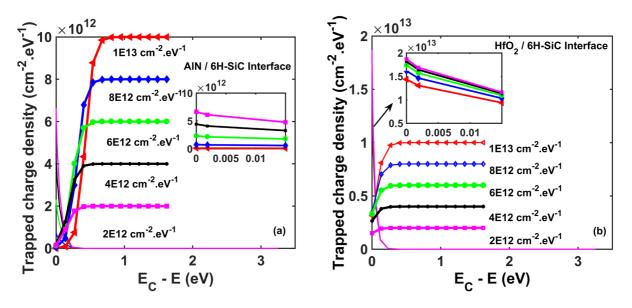


Fig. 3. Trap distribution versus band gap energies of (a) AlN/6H-SiC and (b) HfO₂/6H-SiC interface.

The uniform energetic distribution of traps for a given concentration N_o is given by E_o -0.5 E_s < E < E_o +0.5 E_s , whereas for exponential it is N_o exp (-|(E-E $_o$)/ E_s |). Here E_o (Energy-mid) and E_s (Energy-sigma) are the trap parameters in eV (0.8 and 1.6 for uniform distribution, 0 and 0.04 for exponential distribution respectively). With the increase in trap concentration, we can see that the uniform distribution reduces rapidly and move away from the conduction band edge for AlN-SiC interface.

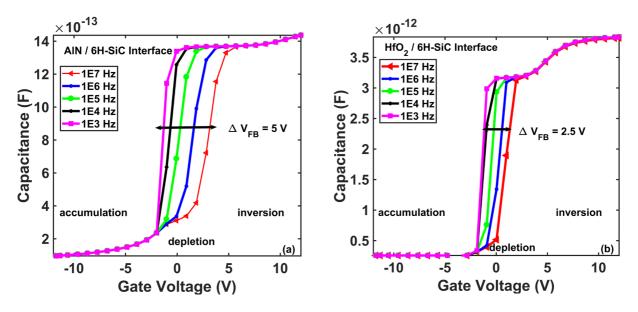


Fig. 4. C-V at different frequencies for (a) AlN/6H-SiC and (b) HfO₂/6H-SiC interface by sweeping gate voltage from -12 V to 12 V.

Fig. 4a and Fig. 4b shows the frequency dependent C-V curves simulated with frequencies ranging from 1 kHz to 10 MHz for AlN/SiC and HfO₂/SiC interface respectively. The shift in C-V curves from depletion to accumulation with respect to voltage is more in case of AlN-SiC interface compared to HfO₂-SiC interface for the frequency range considered. In other words, the frequency has less influence on the flat band voltage shift for HfO₂-SiC interface.

Conclusion

Two-dimensional physics-based simulation of a 6H-SiC MOS capacitor for Pd/AlN/SiC and Pd/HfO₂/SiC interface has been presented. Results have shown that the change in the C-V characteristics of HfO₂/SiC is very steep without degradation in accumulation when compared with AlN/SiC interface. The voltage shift for frequency range (1 kHz - 10 MHz) is comparatively less in HfO₂/SiC interface than AlN/SiC interface. Therefore, a 6H-SiC MOS capacitor with Pd/HfO₂/SiC interface is recommended over Pd/AlN/SiC for detection of hydrogen at higher temperatures, over 700 K.

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