A Physical Model of the Abnormal Behavior of Hydrogen-Terminated Diamond MESFET

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***Abstract* — Hydrogen-terminated Diamond MESFET exhibits abnormal gate capacitance-voltage (CV) relationship, with an insulator barrier-like plateau followed by an abrupt increase in capacitance at large gate bias. A new model is proposed by assuming inhomogeneous band gap in the Interfacial Layer (IL). With this model, various experimental gate CV, as well as gate leakage curves can be matched well with TCAD simulations. This model also offers possible explanation of the double-bumps in transconductance measurements in some experiments.**

Keywords—Hydrogen-terminated Diamond, MESFET, CV, TCAD, Simulation, Interfacial Layer, RF, Power

I. Introduction

Diamond is an ideal material for power and radio frequency applications due to its wide band gap (5.5eV), high hole mobility (1200cm^2/Vs) and high thermal conductivity (22W/cm·K) [1]. However, activation of dopants in diamond is generally difficult due to their large ionization energies (e.g. B has activation energy of 0.36eV) [1]. Surface Hydrogen-terminated diamond (H-Diamond) provides an alternative, in which high areal density (p_s = 10^{13} to 10^{14}cm^{-2}) of Two-Dimensional Hole Gas (2-DHG) can be induced at the surface, despite the reduction of mobility to ~<100cm^2/V·s [2][3]. High performance H-terminated MESFETs have been demonstrated [3].

However, H-terminated diamond MESFETs sometimes exhibit abnormal behaviors that are not well understood. Firstly, in capacitance-voltage (CV) measurements, the Schottky gate contact exhibits an insulator barrier-like plateau followed by an abrupt increase in capacitance at large gate bias [4][5]. Secondly, there are double-bumps in transconductance (g_m) measurements [2][3], which are only possible in dual channel devices. Kasu et al. tried to explain it as the hole penetration through the Interfacial Layer (IL) barrier [6]. However, this is not compatible with the general expectation, that gate leakage will be much higher than the experimental values. Zhou et al. were able to fit experimental CV with their new model but it appears that structure (MISFET) different from the experiment (MESFET) was used in the simulation [7].

Based on the ideas proposed in [6] and [7], in this paper, we present a new physical model to explain the phenomena and demonstrate good matching to experimental Schottky gate CV and leakage (AC and DC), from two different research groups, in the regimes of interest, through TCAD simulations [8].

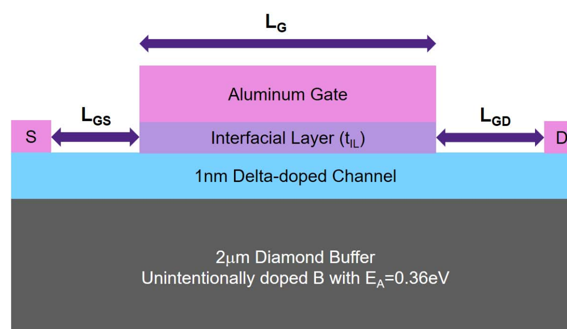

Fig.1. Structure used in the simulations. Experimental values of buffer doping, IL thickness t_{IL}, L_G, L_{GS} and L_{GD} are used in the corresponding simulations.

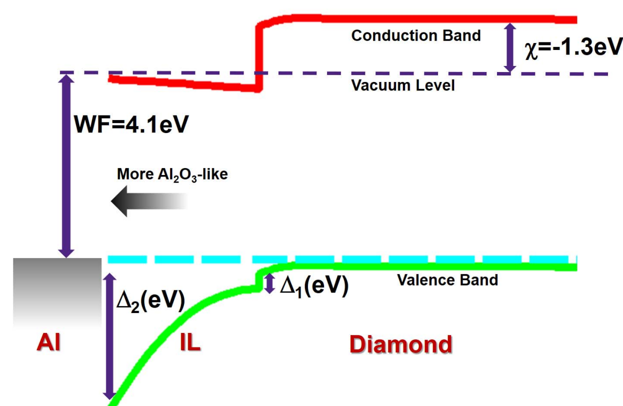

Fig. 2. Band diagram cutting vertically under the Al gate at zero bias, illustrating the setup of the new model. H-diamond with Negative Electron Affinity = -1.3eV is used [1].

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II. MODELING

Fig. 1 shows a typical H-terminated diamond MESFET structure. It is believed that an interfacial layer (IL) is generally formed between the Schottky gate metal (Aluminum) and H-Diamond in a MESFET [2][4][5]. Such layer is about several nm's (t_{IL}) in thickness as found in TEM pictures [5]. Therefore, Schottky contacts in H-Diamond should be modeled with an IL as shown in Fig. 1.

However, with a homogenous IL, one cannot explain the two phenomena mentioned. We therefore postulate that the interfacial layer is composed of varying effective bandgap and thus varying valence band (VB) offset to the VB of diamond (Fig. 2). The VB offset increases from IL/diamond interface to Al/IL interface. This postulation is justified by the facts that 1) thin aqueous wetting layer is believed to exist at the H-Diamond surface to induce 2DHG [1][9] and 2) SIMS data show high Al and O concentration at the Al/IL interface [5]. So, we further postulate that near the IL/diamond interface, the IL "VB" is due to the Highest Occupied Molecular Orbital (HOMO) in the wetting layer [1] and near Al/IL interface, the IL "VB" has strong characteristics of the VB of Al_2O_3. Therefore, the bandgap of IL is chosen to increase quadratically from ~4.5eV at the IL/diamond interface to that of Al_2O_3 (~7.2eV) at the Al/IL interface (Fig. 2). E_g ~ 4.5eV at the IL/diamond interface was chosen because it gives the best fitting.

The main fitting parameters of this model are the VB offset between diamond and IL (Δ_1) and the offset between the Fermi level of Al gate and the IL VB (Δ_2).

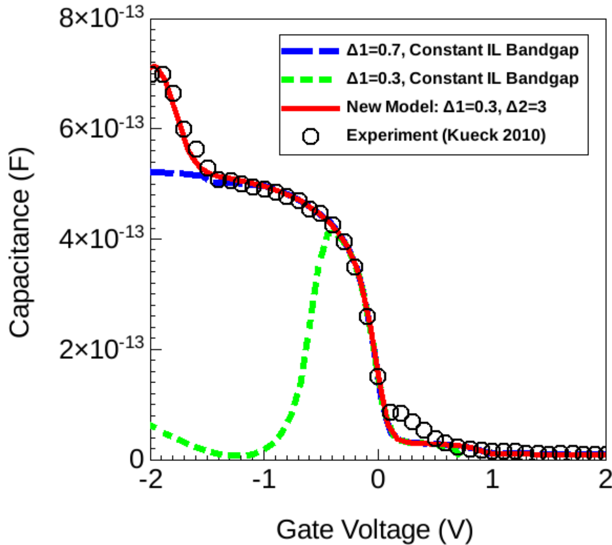

Fig. 3. Experimental [4] and simulated CV's with p_s=1.1×10^{13}cm^{-2}, t_{IL}=3.9nm, L_G=0.8µm and W_G=50µm. Measurement frequency is 1MHz.

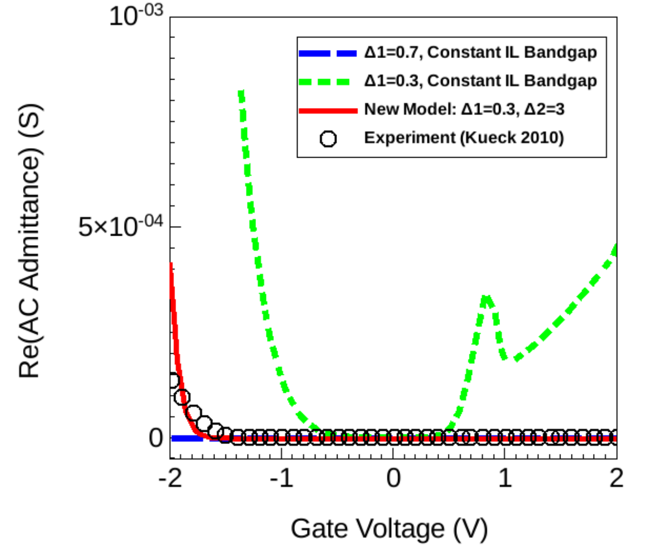

Fig.4. Experimental [4] and simulated real part of AC admittance measurement under the same condition as in Fig. 3.

III. SIMULATION SETUP

In the simulations, Al gate has work function (WF) of 4.1eV. The 2DHG is induced by delta doping at the IL/Diamond interface to give areal concentration of the values given by the corresponding experimental data. In order to match the experimental threshold voltage, fixed charge (Q_F) is added at the IL/Diamond interface under the Al gate. Since the IL/Diamond under and outside Al gate underwent different processing steps, it is reasonable to assume they have different amount of fixed charge.

The diamond buffers are boron doped with concentration based on the values given in the experiment with activation energy = 0.36eV and is simulated with incomplete ionization model.

Fermi-Dirac statistics and mobility high field saturation models calibrated to experimental data were used [10]. Poisson equation, electron and hole continuity equations and hole tunneling (using WKB) at gate are solved self-consistently. Hole tunneling mass = 0.8m_0 was used in all simulations, where m_0 is the free electron mass.

IV. SIMULATION RESULTS

We firstly simulated the MESFET reported by Kueck et al. which has L_G = 0.8µm and W_G = 50µm [4]. Fig. 3 shows the experimental and simulated CV curves, with 2DHG areal density p_s = 1.1×10^{13}cm^{-2}, IL dielectric thickness t_{IL} = 3.9nm and measurement frequency f = 1MHz. p_s and t_{IL} values were based on the data given in [4]. IL dielectric constant is found to be 6.5 to match the

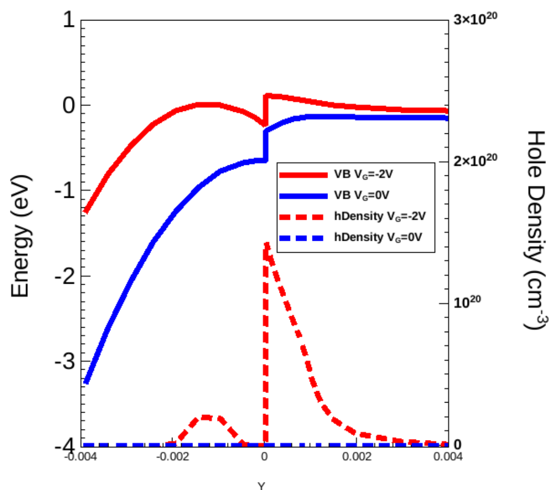

Fig.5. Valence band edge profiles and hole carrier density distributions at V_G=0V or V_G=-2V using the new model. IL/Diamond interface is at Y=0.

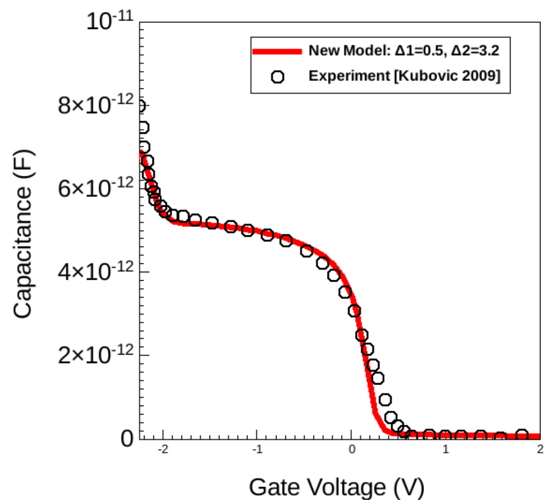

Fig. 7. Experimental [5] and simulated CV curves with p_s=1.1×10^{13}cm^{-2}, t_{IL}=5nm, L_G=5µm and W_G=100µm. Measurement frequency is 1MHz.

experimental capacitance value. Q_F = 1.35×10^{13}cm^{-2} was used to match the threshold voltage. With the proposed model, the plateau and the abrupt increase at V_G ~ -1.5V can be properly captured with Δ_1 = 0.3eV and Δ_2 = 3eV. On the other hand, if homogenous IL is assumed, either the abrupt increase was not captured (Δ_1 = 0.7eV case) or the leakage is too large and gives wrong C-value (which is expected to also appear in experiment when leakage is large) at high negative gate bias (Δ_1 = 0.3eV case).

Fig. 4 shows the real part of simulated and experimental [4] admittance in a CV measurement, which is a strong function of gate leakage. The new model properly captures the abrupt increase of the AC conductance at V_G ~ -1.7V as in experiment. However, for constant IL bandgap, when Δ_1 = 0.3eV is used, the

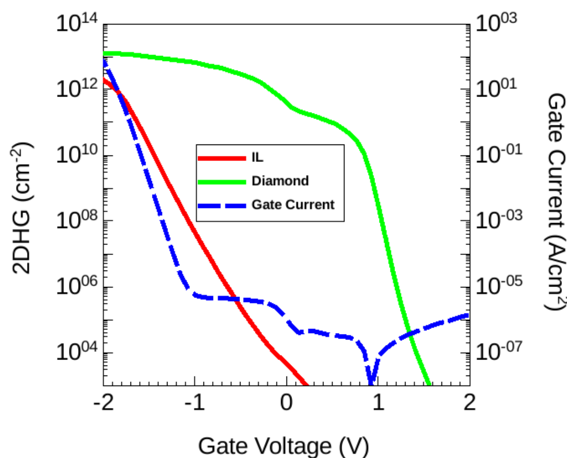

Fig. 6. Simulated gate leakage current and 2DHG in IL and Diamond as a function of gate voltage of the structure in [4].

leakage current is too large resulting in erroneous AC admittance.

Fig. 5 shows the VB profiles and hole distributions at V_G = 0V and -2V. It is evident that holes accumulate inside IL at high bias due to the inhomogeneity of IL bandgap, and a second conduction channel is formed, which is the origin of the abrupt increase in capacitance in CV measurements. From the band diagram, it can be seen that the formation of the second conduction channel is due to the quadratic increase in the bandgap of IL. Moreover, if Δ_1 and Δ_2 are too small, the gate leakage will be excessive. When Δ_1 is too large, there will not be enough hole accumulating in the IL second channel and thus there will be no abrupt increase in capacitance.

Fig. 6 shows the simulated gate leakage and the 2DHG areal densities in diamond and IL as a function of gate voltage. It can be seen that hole starts populating in IL after V_G = -1.2V and reaches almost 2×10^{12}cm^{-2} at V_G = -2V.

V. Additional Verifications

By using the same model, experimental data [5] from another research group was fitted, in which p_s = 1.1×10^{13}cm^{-2}, t_{IL} = 5nm, L_G = 5µm, W_G = 100µm and f = 1MHz. IL dielectric constant = 6.5 was used which gives the best fitting. This is different from the extracted value (5.7) in the original paper because of different extraction methodologies. Q_F = 1.1×10^{13}cm^{-2} was used to match the threshold voltage. Fig. 7 shows the experimental [5] and simulated CV. By adjusting only Δ_1 to 0.5eV and Δ_2 to 3.2eV, the simulated result matches not only the CV but also the DC gate leakage well (Fig. 8) in the regime of

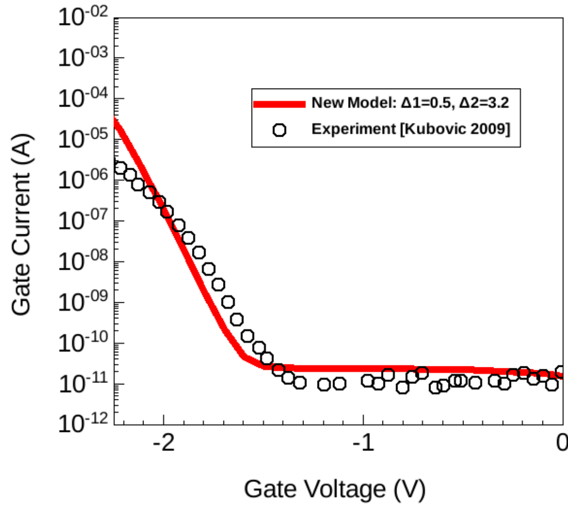

Fig. 8. Experimental [5] and simulated DC gate leakage using the same structure in Fig. 7

interest. Since IL is unintentionally formed without well-controlled conditions, it is reasonable to have different Δ_1 and Δ_2 in different fabrication processes.

It is important to verify that the proposed model has no unphysical effect to other type of simulations. By including the proposed model, the I_D-V_G curve of H-Diamond MESFET from yet another research group [2] is fitted successfully as showed in Fig. 9.

The device has L_G=0.5µm, L_{GS}=1µm, L_{DS}=1.5µm, W=50µm and V_D=-6V. Δ_1 and Δ_2 are 0.3eV and 3eV respectively. Q_F = 0.8×10^{13}cm^{-2} was used to match the threshold voltage. Low hole field mobility is 80cm^2/V·s with saturation velocity = 1.1×10^7cm/s.

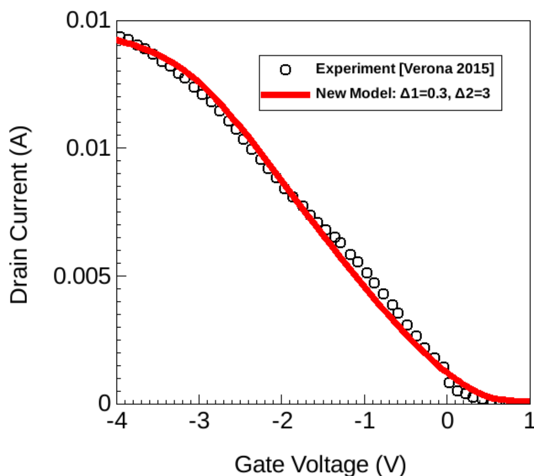

Fig. 9. Experimental [2] and simulated I_D-V_G. L_G=0.5µm, W=50µm, L_{GS}=1µm, L_{DS}=1.5µm and V_D=-6V.

VI. Conclusion

A new model for H-Diamond Schottky contact is proposed and verified with TCAD simulations. It is assumed that the IL has bandgap increasing quadratically from about 4.5eV at the IL/diamond interface to about 7.2eV (that of Al_2O_3) at the Al-gate/IL interface. The main fitting parameters are the VB offset between IL and Diamond (Δ_1) and the offset between the fermi level of Al gate and IL VB (Δ_2). By varying Δ_1 and Δ_2, it can explain and fit experimental results of the abnormal behaviors in CV curves from several different research groups. It also predicts the formation of dual channels, which can be used to explain the double-bumps in some g_m measurements based on the speculation in [2].

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