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Simulation of Direct Tunneling Current in Metal/Gd_2O_3/n-GaN Devices with Nanometer-Thick Gd_2O_3 Layers by Using Self-Consistent Solution of Schrödinger-Poisson Equation

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Abstract *The potential profile of the metal/ Gd_2O_3/n-GaN MOS diode is obtained by solving the Schrödinger-Poisson self-consistently. The finite difference method was implemented to the coupled Schrödinger-Poisson. The tunneling current density through the Gd_2O_3 layer was also calculated. It is found that the tunneling current densities are 1 and 10^3 A/cm^2 for t_{ox}= 2.5 and 2 nm, respectively, at V_{ox}= 1 V.*

Keywords *MOS, Poisson-Schrödinger equation, Gd_2O_3, GaN, Self-consistent solution*

I. INTRODUCTION

A metal-oxide-semiconductor (MOS) structure is the most important device in semiconductor physics [1] This structure has been extensively studied because it is directly related to most common planar devices and integrated circuits [2]. Silicon dioxide films have been used as the gate dielectric since the birth of integrated circuit. In order to achieve the characteristics of the higher speed, greater density, and lower power, each individual device has to be reduced in size. The traditional SiO_2 dielectric faces a number of problems and challenges as the size of the device is scaled down. However, the fundamental limit of ultra thin oxide films is the direct tunneling (current) which grows exponentially with the decrease of film thickness. To overcome this problem, the conventional SiO_2 is replaced by a material with a higher dielectric constant in order to increase the physical thickness of the film, while the "equivalent" electrical thickness with respect to pure SiO_2 and the direct tunneling would be much reduced. Gadolinium dioxide (Gd_2O_3) has the value of dielectric constant high enough to be considered as an alternative gate dielectric [3].

An accurate description of MOS devices requires careful modeling of inversion and accumulation layers at the semiconductor-oxide interface. The importance of quantum effects in inversion and accumulation layers is well known. Some forms of electrically erasable programmable memories employ such tunneling [4]. Some approaches to calculate the gate tunnel currents are the Wentzel-Kramers-Brillouin (WKB) approximation and the self-consistent solution of the coupled Schrödinger-Poisson equation. For practical applications, it is preferred to use the WKB approximation due its simplicity. However, the gate tunnel current calculated by employing the WKB approximation cannot reproduce the measured current at oxides voltages less than 1 V [5].

In this paper, we model the accumulation layer of an n-type GaN-based MOS device by solving the coupled

Schrödinger-Poisson equation self-consistently. The direct tunneling current through the Gd_2O_3 insulator is then calculated.

II. THEORETICAL MODEL

Potential profile of MOS diode for n-type semiconductor at the accumulation case (a positive bias is applied to the metal gate) is shown in Figure 1. The behavior of an electron in the accumulation layer is described by the time independent Schrödinger equation. For an electron residing inside the potential well of the n-type GaN semiconductor near to the interface, its energy will experience quantization and this condition is referred as bound states. The Schrödinger equation to be solved is given by:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x). \quad (1)$$

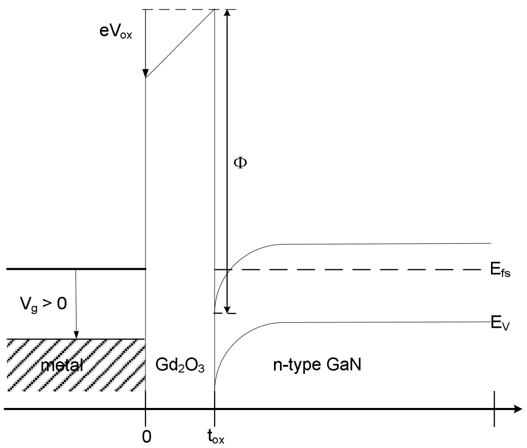

Fig. 1. Potential Profile of the MOS diode in the accumulation mode.

The electron energy and wave function are obtained by applying the boundary conditions at x = 0 and L and the continuity of ψ and $\frac{1}{m}\frac{d\psi}{dx}$ as follow [4]:

$\psi(x = 0) = \psi(x = L) = 0,$ (2.a)

$\psi(x = t_{ox}^-) = \psi(x = t_{ox}^+),$ (2.b)

$$\frac{1}{m_{Gd_2O_3}}\frac{d\psi(x=t_{ox}^-)}{dx}=\frac{1}{m_{GaN}}\frac{d\psi(x=t_{ox}^+)}{dx}, \quad (2.c)$$

where m_{Gd2O3} and m_{GaN} are the electron effective masses in the Gd_2O_3 and GaN, respectively.

The Poisson equation to be solved in obtaining the potential $V(x)$ is:

$$\frac{d^2V(x)}{dx^2}=-\frac{\rho(x)}{\varepsilon}, \quad (3)$$

where ε_{GaN} is the permittivity of GaN. The total charge density, ρ(x), is [4]:

$$\rho(x)=eN_D-e\sum_j N_j\left|\psi_j(x)\right|^2. \quad (4)$$

Here e is the electronic charge and N_j the doping concentration. Electron concentration in each quantization level j is given by:

$$N_j=\frac{n_v m_d kT}{\pi\hbar^2}\ln\left(1+\exp\left[\frac{E_{fs}-E_j}{kT}\right]\right), \quad (5)$$

where n_v = 1 is the degeneracy, m_d the density of states mass, k the boltzman constant, T the temperature, E_{fs} the Fermi energy of GaN and E_j the energy associated with the quantization level j. The potential in Eq. (3) fulfills the following conditions:

$$\varepsilon_{Gd_2O_3}\frac{dV(x=t_{ox}^-)}{dx}=\varepsilon_{GaN}\frac{dV(x=t_{ox}^+)}{dx}. \quad (6)$$

The self consistent calculation starts using equations in the form as intial guess potentials:

$V(x)=\alpha x+c$, for $0\le x\le t_{ox}$ (7a)

$V(x)=\beta(1-\gamma\exp(-\delta))-\zeta$, for $t_{ox}\le x\le L$ (7b)

where α, β, γ ,δ,ζ and c are constants chosen empirically to give the best result. The initial guess is substituted into Eq. (1) to get E and ψ. The obtained E and ψ is then substituted into Eq. (5) to get N_j and $\rho(x)$. After that, Eq. (3) is solved to get new potential $V(x)$. The potential obtained from the Poisson equation is compared with the potential used in the Schrödinger equation. This process is done repeatedly until convergent.

The tunneling current J due to the bound states is [4]:

$$J = e\frac{n_v m_d kT}{\pi\hbar^2}\ln\left[\frac{1+Exp\left(\frac{E_{fm}-E_j}{kT}\right)}{1+Exp\left(\frac{E_{fs}-E_j}{kT}\right)}\right]\frac{1}{\tau_j}. \qquad (8)$$

The lifetime τ_j is approximately given by:

$$\frac{1}{\tau_j} = \frac{D(E_j)}{\int_0^{xj}\sqrt{2m/[E_j - E_c(x)]}dx}, \qquad (9)$$

where $D(E_j)$ is the tunneling probability through the oxide layer and x_j the position where E_j crosses the conduction band $E_c(x)$.

III. RESULTS

In order to obtain the potential profile and calculate the tunneling current, the following parameters were used: m_{Gd2O3}= 0.29 m_o, m_{GaN}= 0.2 m_o, Φ= 1.42 eV, ε_{Gd2O3}= 14.2 ε_o, ε_{GaN}= 10.4 ε_o, T= 300 K, and concentration doping of the substrate is 10^{23} m^{-3}. The software utilized in this simulation was Matlab version 6.5. The finite difference method was implemented in the calculation of the coupled Schrödinger-Poisson.

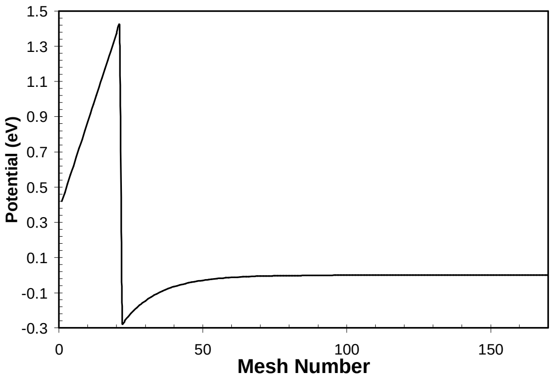

Fig. 2. Potential profile of MOS diode at V_{ox}= 1V and t_{ox} = 2 nm.

The potential profile of the n-GaN-based MOS device with the 2 nm-thick Gd_2O_3 layer and oxide voltage V_{ox}= 1V, which was obtained by solving the coupled Schrödinger-Poisson self-consistently, is shown in Fig. 2.

Figure 3 depicts the tunneling current density as a function of the oxide voltage. It is shown that at V_{ox}= 1 V, the tunneling current densities are 1 and 10^3 A/cm^2 for t_{ox}= 2.5 and 2 nm, respectively.

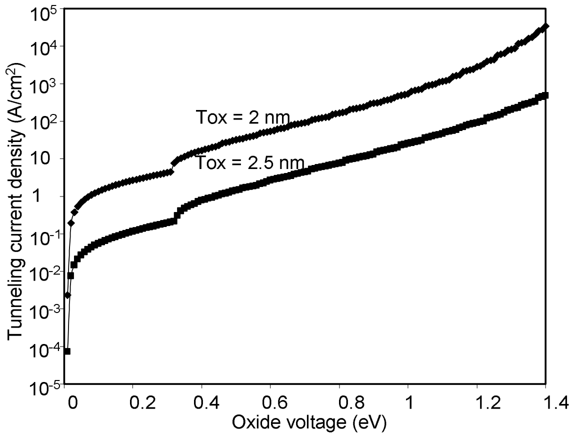

Fig 3. Simulated tunneling current densities for t_{ox} = 2 nm and 2.5 nm

IV. SUMMARY

The potential profile of the n-GaN-based MOS diode has been obtained by solving the Schrödinger-Poisson self-consistently. The tunneling current density through nanometer-thick Gd_2O_3 layer has also been calculated. It is found that the tunneling current densities are 1 and 10^3 A/cm^2 for t_{ox}= 2.5 and 2 nm, respectively, at V_{ox}= 1 V.

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