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Impact of bandstructure effects in III-V nMOSFETs

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***Abstract*—In this work, Poisson-Schrödinger simulations of thin channel nMOS capacitances with a III-V channel are presented, which include both the non-parabolicity correction, and the bandstructure modification through an empirical modification of the effective mass. These simulations are first validated against simulation and experimental data reported in the literature. Then they are employed to evaluate quantitatively the impact of quantum effects on III-V devices. Finally a simple compact model is proposed to evaluate the inversion charge of InGaAs channels in Double-Gate MOSFETs.**

1. Introduction

The III-V materials are potential candidates for sub-7 nm node thanks to their high injection velocity [1]. However, their low density of states (DOS) is expected to deteriorate their performance due to the enhanced Dark Space (DS) [2]. Fortunately, the strong non-parabolicity (NP) of the bandstructure in III-V materials, and the increase of the effective mass in thin channels, may help to alleviate this issue. In this work both these aspects will be included in Poisson-Schrödinger (PS) simulations, in order to evaluate quantitatively how the DOS of $In_{0.53}Ga_{0.47}As$ may impact the MOSFET performance. Finally, a simple compact model for the inversion charge will be proposed for Double-Gate devices.

2. Simulations description and validation

The non-parabolicity model reported in [3] is employed here. Its implementation is validated by comparison with the UTOX simulator results [4], where the same non-parabolic model has also been employed (Fig. 1a). The bandstructure modification in thin films is represented by a modification of the effective mass used in the simulator. Using Vegard's law, the following expressions were found sufficient to reproduce the Tight-Binding (TB) results reported in [4], [7] for the in-plane mass: $m_{\Gamma,//} = m_{\Gamma,0} \cdot (1 + 2.93\,\mathrm{nm}/t_{ch})$ and the confinement mass: $m_{\Gamma,c} = m_{\Gamma,0} \cdot (1 + 6.9\,\mathrm{nm}/t_{ch})$ ($m_{\Gamma,0}$ being the bulk effective mass of the Γ valley in $In_{0.53}Ga_{0.47}As$). As shown in Fig. 1b, the PS simulations reproduce well the experimental gate capacitance values reported in [5]. The improved accuracy of the NP simulations compared with the parabolic one (dashed line labeled "PS parabolic") is also clearly visible in Fig. 1b. Interface traps must be included to reproduce the experimental values reported in [6]. As in bulk [8], a linear trap density (with a slope $d_{it} = \mathrm{d}D_{it}(E)/\mathrm{d}E$ starting at energy $E_{off} = 300$ meV above threshold) is introduced in the simulations for that aim.

3. Impact on III-V MOSFET characteristics

The threshold voltage shift induced by quantum effects (ΔV_{th}) in a Double Gate (DG) nMOSFET is plotted in Fig. 1d for the different bandstructure models considered: parabolic with $m_{\Gamma,//} = m_{\Gamma,c} = m_{\Gamma,0}$ (labeled "para."), non-parabolic with $m_{\Gamma,//} = m_{\Gamma,c} = m_{\Gamma,0}$ (labeled "NP"), and non-parabolic with $m_{\Gamma,//}(t_{ch})$ and $m_{\Gamma,c}(t_{ch})$ fitted on TB results as explained in sec. 2 (labeled "NP+m*(TB)"). The Si parabolic simulation results are also depicted in Fig. 1d for the sake of comparison. Although ΔV_{th} for InGaAs is much larger than the Si values in parabolic simulation using the bulk effective mass ($m_{\Gamma,0}$), this difference almost completely vanishes when both the NP correction and the effective mass from TB models are included. As a result, the V_{th} variability induced by quantum effects (which is a major concern for III-V materials [9]) is strongly attenuated compared with parabolic simulations (Fig. 2a), almost matching Si values. Finally, the loss of density in inversion is also alleviated, as evidenced when the gate workfunction is aligned in each case to provide the same density below threshold (Fig. 2b). Naturally the DS is also reduced in comparison with parabolic simulations (Fig. 2c). It is noteworthy that the DS of InGaAs in parabolic simulations below $7 \cdot 10^{12}$ cm^{-2} is much larger than its bulk

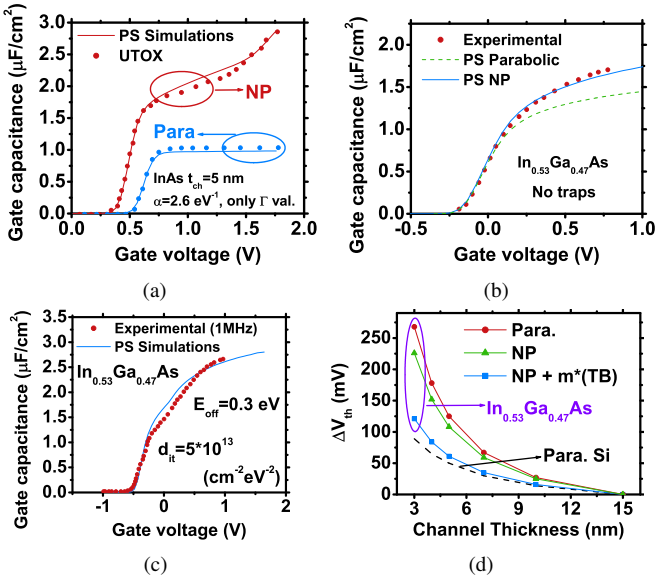

Fig. 1: a) Comparison with UTOX. b) Comparison with experimental data reported in [5] and (c) in [6]. d) Threshold voltage shift (ΔV_{th}) in a DG MOSFET.

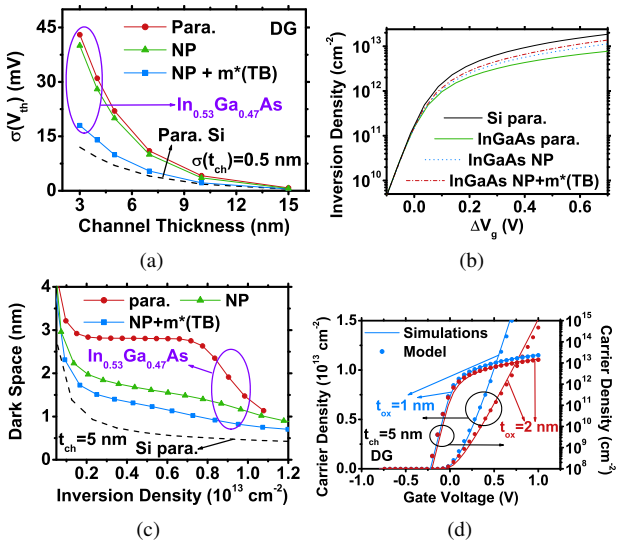

Fig. 2: a) Standard deviation of the threshold voltage $\sigma(V_{th})$ considering a Gaussian distribution of the channel thickness $\sigma(t_{ch})$= 0.5 nm. b) Comparison of the inversion surface densities obtained with the different bandstructure models. c) DS obtained by DS=$(\epsilon_{ox}/C_g - t_{ox})$, where C_g is the gate capacitance and t_{ox} the oxide thickness. d) Comparison of the charge model using eq. (1) with the PS results for $t_{ch} = 5$ nm.

value. Actually the equivalent semiconductor thickness (i.e $DS{\cdot}\epsilon_s/\epsilon_{ox}$, where ϵ_s and ϵ_{ox} are the semiconductor and oxide dielectric constants) is even larger than the channel thickness (t_{ch}). This is explained by the quantum capacitance effect [10], [2], which prevents the gate capacitance from reaching the oxide capacitance C_{ox}, even if the charge centroid is reduced by shrinking t_{ch}. The "capacitive" value of DS may thus differ significantly from the charge centroid in thin-film devices.

4. Inversion charge model

As in the bulk case [8], the inversion charge model is based on the UCCM equation [11]: $V_g = V_{th} + \phi_t \ln(N_s/N_{th}) + q(N_s - N_{th})/(2C_{inv})$, where q is the electron charge and ϕ_t the thermal voltage. N_s is the inversion surface density, and N_{th} its value at threshold. In [8], the centroid of charge was employed to evaluate the inversion capacitance C_{inv}. This approach is however not possible in thin-film devices, because the DS is not necessarily equal to the centroid of charge, as pointed out in sec. 3. An empirical expression of the capacitive equivalent thickness (t_{inv}) is therefore employed to evaluate C_{inv}:

$$t_{inv}(N_s) = t_{ox} + \frac{\epsilon_{ox}}{\epsilon_{ch}}\left[0.36t_{ch} + \frac{t_{q0}m_0/m_{\Gamma,//}(t_{ch})}{1+3\alpha k_bT(N_s-N_{th})/N_{th}}\right]\cdot\frac{1}{1+\left[\tanh\left(\frac{t_{ch}}{4\,\mathrm{nm}}\right)\right]^4} \quad (1)$$

In (1), the term $\propto t_{ch}$ represents the charge centroid effect [2], and the term $\propto t_{q0}m_0/m_{\Gamma,//}(t_{ch})$ represents the quantum capacitance effect [2] (t_{q0}=7 nm). The term $(1+3\alpha k_bT(N_s-N_{th})/N_{th})$ represents the NP DOS increase

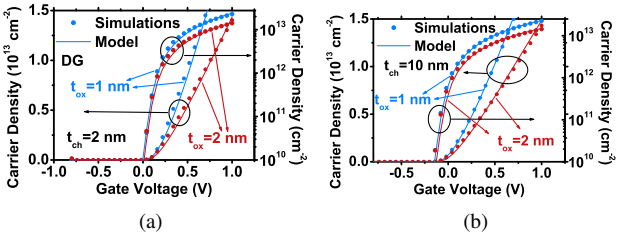

Fig. 3: Comparison of the charge model using eq. (1) with the PS results for (a) $t_{ch} = 2$ nm and (b) $t_{ch} = 10$ nm.

in inversion (in contrast to the parabolic case, where the DOS remains constant once the 2D Fermi-Dirac statistics is degenerated). The factor $\left(1+\left[\tanh\left(\frac{t_{ch}}{4\,\mathrm{nm}}\right)\right]^4\right)$ represents the occupation of the second subband for thick channels, which reduces both the charge centroid and the quantum capacitance. This factor is independent of the gate voltage, as no attempt is made to match the step like behavior of C_g obtained in parabolic simulations [12], which is strongly attenuated by the non-parabolicity, and has not been experimentally observed so far at room temperature (unless satellite valleys are occupied, which is not the case for the moderate overdrive voltages considered here). The inversion charge obtained using (1) features an acceptable accuracy, as shown in Fig. 2d, 3a and 3b.

5. Conclusion

The impact of DOS and bandstructure on InGaAs MOSFET inversion charge has been investigated with Poisson-Schrödinger simulations including both non-parabolicity and modification of the bandstructure. It was found that the characteristics of InGaAs MOSFETs (threshold voltage and gate capacitance) may actually be much less severely impacted by quantum effects than the parabolic simulations may suggest, hence tempering the performance degradation expected due to the DOS bottleneck. Finally, a simple inversion charge compact model including all these effects has been proposed, which matches the PS results.

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