Accumulation capacitance of narrow band gap metal-oxide-semiconductor capacitors

Erik Lind,1,a Yann-Michel Niquet,2 Hector Mera,2 and Lars-Erik Wernersson1,3

1Solid State Physics, Lund University, Box 118, 22100 Lund, Sweden
2CEA-UJF, INAC, SP2ML_SIM, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France
3Electrical and Information Technology, Lund University, Box 118, 22100 Lund, Sweden

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We have investigated the accumulation capacitance-voltage characteristics for capacitors with narrow band gap materials using modeling and experiments. The capacitance for InAs and In0.53Ga0.47As capacitors with a HfO2 oxide layer has been calculated using atomistic tight-binding, effective mass, and semiclassical nonparabolic models. The simulations show that band structure effects have a strong influence on the accumulation capacitance, and are essential for the description of narrow band gap capacitors. The calculated tight binding data compare well with measurements on n-type InAs HfO2 capacitors on (100) and (111)B substrates, highlighting the nonparabolicity as the main origin for the large accumulation capacitance. © 2010 American Institute of Physics.

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The performance of metal-oxide-semiconductor (MOS) field-effect-transistors can potentially be enhanced by using narrow band gap III–V semiconductors as the channel material.1–3 In this context, capacitance-voltage (CV) measurements on MOS capacitors (MOSCAPs) are an important tool used to characterize the physical properties and quality of the III–V semiconductor interface.4 The CV data are usually interpreted through comparisons with simulations based on the effective mass approximation. There is currently a strong interest in MOS field-effect-transistors and MOSCAPs based on narrow band gap materials, such as InAs (Refs. 5 and 6) and In0.53Ga0.47As (x > 0.5).7,8 However, the interpretation of CV data is not straightforward in narrow band gap MOSCAPs with thin, high-κ oxides. This is mainly due to quantum confinement, and to the strong nonparabolicity of the conduction band.9 Indeed, the conduction band effective mass tends to be small in narrow band gap materials, which leads to small density of states and semiconductor capacitances. For a MOSCAP biased in the strong accumulation regime, the Fermi level can therefore rise high above the conduction band edge. Thus, nonparabolicity effects must be taken into account to avoid large errors in the calculated capacitances, which can make data interpretation difficult. The small conduction band effective mass can further lead to strong quantum quantization, especially in the accumulation region, where the charge carriers are confined at the semiconductor-oxide interface.

In this letter, we compare experimental CV data from n-type InAs high-κ MOSCAPs, with capacitance calculations using a sp3d5s* tight binding (TB) model, a semiclassical nonparabolic model (SCNP),9 an effective mass Schrödinger–Poisson solver (EM), and a semiclassical effective mass approximation (SCEM). It is clearly shown that the effective mass models underestimate the semiconductor accumulation capacitance with respect to the TB and SCNP calculations. Quantum effects are shown to be substantially smaller in the accumulation region than nonparabolicity effects. The TB model shows very good agreement with our measured data from InAs MOSCAPs with various substrate orientations and oxide thicknesses.

MOSCAPs were fabricated on (100) and (111)B InAs wafers with nominal n-type doping Nn=3.0×1015 cm−3 and Na=7.0×1016 cm−3, respectively. The samples were etched for 1 min using HCl:H2O (1:1) and rinsed in 2-isopropanol for 20 s, then loaded into a Cambridge Nanotech Savannah-100 atomic layer deposition system. 2.5 and 6-nm-thick HfO2 films were grown using 35 cycles and 80 cycles, respectively, of tetraakis(dimethylamido)hafnium and H2O, at a deposition temperature of 250 °C. The relative dielectric constant of the deposited HfO2 is 21 ± 2, as obtained from measurements of reference HfO2 diodes on n-type Si. The HfO2 thickness was calibrated through reference thickness series depositions on Si, and subsequent thickness determination using a variable angle spectroscopic ellipsometer. This leads to nominal oxide capacitances Cox=31 ± 3 fF/μm2 for the 6 nm samples and Cox=81 ± 7 fF/μm2 for the 2.5 nm sample. W/Au contacts with areas of 2560 μm2 were formed using dc sputter deposition, optical contact lithography, and etching. CV data was then obtained at an oscillation amplitude of vosc=30 mV, at frequencies between f=100 kHz and 35 MHz, using an Agilent 4294A impedance analyzer and a Cascade 11000B shielded probe station. The measurement temperature was T=220 K.

The TB capacitances were computed with a fully atomistic Schrödinger–Poisson solver based on the sp3d5s* TB model of Ref. 10. The density of conduction band electrons is calculated from the band structure and wave functions of a 250-nm-thick semiconductor film sampled over 2400 transverse k points around Γ. By solving Poisson’s equation self-consistently, the total semiconductor charge, Qs, and the semiconductor capacitance, Csc=dQs/dφs, can be calculated as a function of the surface potential, φs. In the accumulation regime, and in the absence of border traps, Cs corresponds to the high-frequency capacitance. For the EM calculations, we also used a self-consistent Schrödinger–Poisson solver, based on the effective mass approximation instead of the tight-binding method. Both the TB and EM approaches describe quantum confinement but only the former reproduces the
nonparabolicity of the conduction band. For the semiclassical SCNP calculations, we followed Ref. 9, which is based on a two-band $k\cdot p$ model. The carrier density in the conduction band is here given by Eq. (1).

$$n(\phi) = \frac{2N_c}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{e(1+ae)(1+2ae)}de}{1+\exp(e-\phi)}.$$  

(1)

Here, $e=(E-E_f)/kT$ is the normalized electron kinetic energy, $\phi=(E_f-E_c)/kT$ is the normalized Fermi energy, and $N_c$ is the effective conduction band density of states. The nonparabolicity factor, $\alpha=(1-m_s/m_0)^2/2\epsilon_s$, is enhanced by a small effective mass $m_s$ and a narrow normalized gap $\epsilon_s=(E_c-E_f)/kT$. For $\alpha=0$, this model reduces to the traditional SCEM with Fermi–Dirac statistics. Neither the SCNP nor the SCEM approach takes quantum confinement into account. We therefore expect the TB model to provide the most accurate results, since it reproduces the full band structure and describes quantum confinement effects.

Figure 1(a) shows the semiconductor capacitances $C_s$ for an InAs MOSCAP, calculated using the TB, EM, SCNP, and SCEM approaches. The doping is $N_d=3.0 \times 10^{16}$ cm$^{-3}$ and the temperature is $T=220$ K. For the SCNP, SCEM, and EM calculations, the parameters are $m_s=0.023 m_0$ and $E_g=0.36$ eV. A surface potential of $\phi=0$ corresponds to flatband condition. We note a striking difference between the parabolic and nonparabolic models. The semiconductor capacitance increases slowly for $\phi$ in the effective mass approximation (SCEM and EM), while it increases almost linearly in the nonparabolic SCNP and TB approaches, due to the faster increase in the density of states with energy for those models. While nonparabolicity increases $C_s$, quantum confinement reduces the density of states and moves the charge centroid away from the semiconductor-oxide interface. This decreases the semiconductor capacitance, as can be seen by comparing the TB and SCNP, and EM and SCEM models, respectively, in Fig. 1(a). The reduction in $C_s$ due to quantum confinement is, however, substantially weaker than the increase due to nonparabolicity, especially for large $\phi$. Thus, nonparabolicity effects must be primarily included for accurate calculations of the capacitance in narrow band gap materials.

Figure 1(b) shows the CV data calculated with the different models, for $C_{ox}=31.6$ fF/μm$^2$. Since $C_g=C_{ox}/(1+C_{ox}/C_s)$, the differences between the calculated $C_g$ are smaller than those between $C_s$. Nevertheless, at $V_g=1$ V the SCEM and EM model underestimate the capacitance by about 50% with respect to the TB model. The SCNP and TB models, which both account for nonparabolicity, are on the other hand in fairly good agreement in the accumulation region.

Figure 1(c) shows the calculated conduction band profile from the TB model at $V_g=1.0$ V. Due to the thin oxide thickness (<6 nm) and large gate bias (1 V), the Fermi level reaches up to about 0.6 eV above the conduction band edge, where band structure effects are significant. This is clearly evidenced in the inset of Fig. 1(c). At this bias, we also observe that only four subbands are occupied below $E_f$. In spite of quantum confinement, the nonparabolic behavior of the conduction band leads to large $C_s$ and $C_g$. We have also performed calculations for an In$_{0.53}$Ga$_{0.47}$As MOSCAP, as shown in Fig. 2. Since the effective mass and band gap of In$_{0.53}$Ga$_{0.47}$As ($m^*=0.041 m_0$ and $E_g=0.76$ eV) are larger than those of InAs, the discrepancies between the SCEM/EM and TB/SCNP models are smaller. Nevertheless, the SCEM model gives capacitances 20% smaller than the TB model at $V_g=1$ V. Thus, for an accurate fit of the accumulation capacitance, the inclusion of band structure effects is important also in In$_{0.53}$Ga$_{0.47}$As MOSCAPs.

Some extraction techniques for the density of interface traps ($D_{it}$), such as the low-frequency and Terman methods.1,7

![FIG. 1. (Color online) (a) Calculated InAs semiconductor capacitance $C_s$ vs surface potential $\phi$, using the SCNP, TB, SCEM, and EM models ($N_d=3.0 \times 10^{16}$ cm$^{-3}$ and $T=220$ K). (b) Calculated InAs CV-data with $C_{ox}=31.6$ fF/μm$^2$ and $N_d=3 \times 10^{16}$ cm$^{-3}$. The inset shows the relation between $C_{ox}$, $C_s$, and total gate capacitance $C_g$. (c) Conduction band profile from the TB model, at a gate bias $V_g=1$ V. The Fermi level (dashed line) is taken as the reference energy. The dotted lines are the subband edges. The inset shows the bulk conduction band structure of InAs in the TB, effective mass (EMA), and two-band $k\cdot p$ approximations.](image-url)
To conclude, we have experimentally and theoretically investigated the accumulation capacitance of narrow band gap III–V MOSCAPs. It is shown that the introduction of nonparabolic effects is necessary to accurately describe the shape of the CV curve. A reasonable fit can nonetheless be obtained in the strong accumulation regime using a simple two-band semiclassical model, disregarding confinement effects.

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FIG. 3. (Color online) (a) Comparison between experimental and TB data for InAs (100) and (111) MOSCAPs with \( t_{\text{ox}} = 6 \) nm and \( C_{\text{ox}} = 31.2 \text{ fF/\mu m}^2 \). (b) Experimental and TB/SCEM data for InAs (100) MOSCAP with \( t_{\text{ox}} = 2.5 \) nm, \( C_{\text{ox}} = 81 \text{ fF/\mu m}^2 \), and \( N_d = 3 \times 10^{16} \text{ cm}^{-3} \).