Modeling study of capacitance characteristics in strained High-K Metal gate technology: impact of $Si/SiO_2/HK$ interfacial layer and band structure model

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Abstract

The importance of developing predictive modeling tools has considerably increased with the diffusion of nanoscale technologies, in which strained layers and heterojunctions determine the materials modeling complexity. A self–consistent Poisson–Schroedinger solver based on a full-band (FB) k.p method has been developed and validated on large test structures, studying the oxide capacitance for various gate stacks. Among the effects governing the electrostatics of the devices, the impact of band structure models of the oxide, of the semiconductor, and the effects of the Si/SiO_2 interfacial layers have been studied. The predictions of FB k.p models are compared a tight binding model and to simpler effective mass approximation (EMA) models. The oxides have been treated as pseudo zinc-blend materials, adjusting the model parameters using ab-initio simulations. The importance of having such accurately calibrated models relies in the reduced computational time of EMA models with respect to FB models. Additionally 2D TCAD simulations have been performed using a commercial simulation package to assess the predictions of these simpler models.

Keywords: Poisson–Schroedinger model, interfacial layer, full-band model, High–K stack.

Introduction

The continuous technology improvements implying the reduction of device size to nanoscale dimensions requires a deep understanding and modeling of nano-scale processes. When complex hetero–structures including strained layers are introduced in the device, understanding nanoscale physical mechanisms and providing accurate predictions becomes critical for reducing technology development costs and improving product yield. All these properties are combined in modern devices where the presence of atomic layers at the interfaces between different materials is becoming more and more important for controlling tunneling leakage currents and dissipated device power.

The models required for the investigations of such complex devices are based on first principles calculations and they are capable of reproducing band structure effects without fitting parameters. However, they are known to be limited to macro-cells simulations and thus they are not suitable for reproducing the electrostatics of the device. On the other hand, simpler and faster models based on effective mass approximations (EMA) can lack of accuracy or scalability, if a correct calibration methodology is not performed. The presence of interfacial layers (IL) formed at the interface between SiO_2 and Si has been intensively demonstrated and studies showed the presence of a non–abrupt compositional and structural transition over a depth of a few Å [1]. The aggressive oxide scaling and the introduction of High-K oxide–stacks have further increased the interest of models taking into account the role and the impact of ILs on electrical characteristics [2].

In this paper, the impact of band structure and interfacial layers on electrical characteristics have been studied using self–consistent 1D Poisson–k.p–Schroedinger (PS) simulations. The importance of having accurately calibrated EMA models has been demonstrated, taking into account quantum and band structure effects for the simulation of complex heterostructures. The test structures and the model validation methodology are described in Section I; in Section II, band structure effects and the impact of strain in the structures are discussed, comparing model results with first principles simulations for extracting critical simulation parameters. Finally, in Section III the effects of IL are detailed with a comparison to 2D TCAD simulations.

I. Model description and validation

A self–consistent 1D Poisson–Schroedinger (PS) solver based on a full-band k.p method within the envelope-function approximation [3] has been developed and validated on large MOSCAP test structures. Multi-Band Models (MBM) and Coupled Multi-Band 6-k.p models (C-MBM) for both semiconductor and oxide materials have been implemented in the simulator for a more insight study of device properties and their impact on the characteristics.

Both Metal/HK/P-Well and Metal/HK/N-Well devices have been integrated and characterized using a HP4284A LCR-meter for oxide capacitance measurements. The stacks are composed by TiN, HfO_2 and

SiO_2 oxide over Si. Two different sets of oxide stacks have been studied varying the thickness of the SiO_2 layer (physical thicknesses t_{SiO2} measured with ellipsometry ranging from 20Å to 35Å). The model has been also validated in the presence of a highly–strained layer (SL) using Si as a buffer in HighK/N-Well devices. Typical comparisons with excellent matching between measurements and simulations are shown in Figures 1 and 2 for different oxide stacks. In both the cases, a 5Å-thick IL has been modeled at the Si/SiO_2 interface, with a gradual linear variation of all the electrical and physical properties of the material. Figure 1 also shows the comparison with 2D TCAD simulations, where quantum, band structure and IL effects are taken into account using fitting parameters.

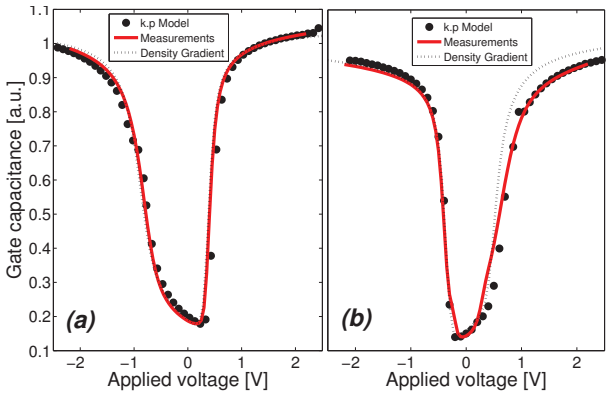

Figure 1: C-V curves on HighK/P-well (a) and HighK/N-well (b) structures with oxide stack having $t_{SiO2} > 35$ Å(symbols: full band k.p model, dashed line: TCAD simulation using density gradient model, continuous line: measurements). The 5Å-thick interfacial layer has been modeled at the interface between SiO_2 and the substrate for both the devices.

II. Band structure effects

Among the effects governing the electrostatics of the devices, the impact of band structure models of both the oxide and the semiconductor have been studied. The investigation of these effects has been carried out using the CV characteristic of the HighK/Nwell device shown in Figure 2(b) as a reference.

Advanced rigorous full band (FB) models are compared to simpler techniques based on MBM EMA models, showing the importance of having an accurate calibrated model to achieve the device electrostatics for faster simulations. Two advanced FB models (sp3d5s* tight binding (TB) model of [4] and 30-bands k.p model from [3]) have been considered. Figure 3 shows the good matching achieved on the band diagram of SiO_2 between the ab-initio, FB and EMA simulations. In the FB models, the oxides have been treated as pseudo zinc-blende

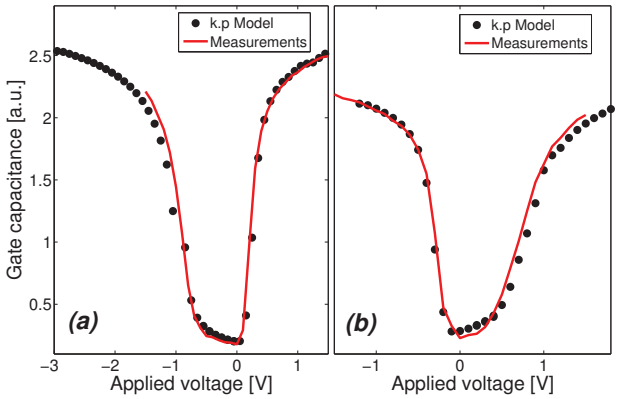

Figure 2: C-V curves on HighK/Pwell (a) and HighK/Nwel (b) structures with oxide stack having $t_{SiO2} < 20$ Å(symbols: full band k.p model, line: measurements). The 5Å-thick interfacial layer has been modeled at the interface between SiO_2 and the substrate.

materials, adjusting the model parameters to match the band structure obtained from first principles [5]. The importance of having accurately calibrated EMA models relies in the reduced computational time of EMA models with respect to FB models.

The results on the device electrostatics of the two advanced models are compared to simpler 6-band k.p and 3-band EMA models (accounting for HH, SO, LH Γ-bands or Δ_X, Δ_Y and Δ_Z bands for electrons and holes respectively). Figure 4(a) shows a comparison between C-V curves simulated in accumulation with a 15-band k.p and a 3-band EMA model for electrons, accounting for strain, heterostructure effects and mass variations [3]. A gradual 5Å-thick interfacial layer is modeled at the SiO_2/Si interface. The importance of modeling band deformation due to strain effects has been justified showing the large differences induced on the CV curve when the strain contribution is removed. Indeed, due to the presence of strain, heterostructure and interface properties, Δ_X and Δ_Y electrons exhibit a large band offset, with respect to the carriers in the Δ_Z valley which remain confined in the buffer. Figure 4(b) shows the impact of FB models and strain on the accumulation charge and on the potential. Also in this case, a good alignment of the three models has been obtained.

In Figure 5(a) the band structure obtained with full band k.p is compared to the one used for 3-band EMA. Also shown in Figure 5(b) is the behavior of the wavefunction penetration into the oxide layer corresponding to the first level of energy of the carriers. The good alignment achieved for the three models, including TB results, confirms the accuracy of the approach.

Similar studies have been performed in inversion, comparing a 30-band k.p, a 6-band k.p and a 3-band EMA for holes considering all Γ-bands [6] and focusing

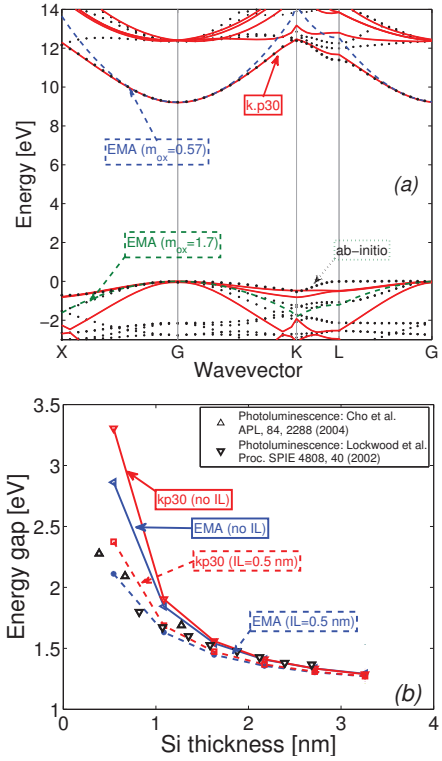

Figure 3: (a) Ab-initio band diagram of the SiO_2 material modeled with a β-cristobalite structure, FB k.p model results using a pseudo zinc-blende structure and EMA model comparison. (b) The relation between Si thickness and energy gap for k.p and calibrated EMA for a Si layer embedded in a SiO_2 buffer.

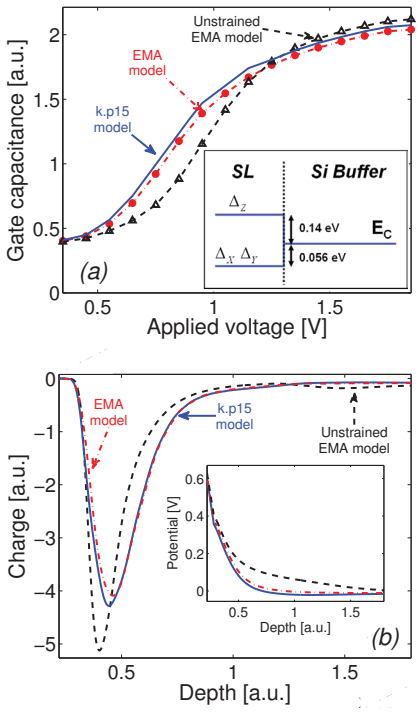

Figure 4: (a) C-V curves comparing a 3-band EMA model and a full band 15-k.p model for electrons in accumulation for device shown in Figure 2(b). In the inset, conduction and valence bands at $V = V_{FB}$. The curve is also compared to simulations on a device where the strain is not taken into account and important changes are observed. (b) Accumulation charge on the same device at $V = 1.85V$, comparing the 15-k.p model with the 3-band EMA model on both strained and unstrained devices.

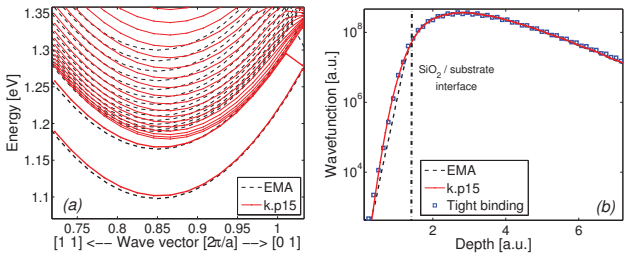

Figure 5: (a) Comparison between the band structures used in 15-k.p and 3-band EMA used for simulations in Figure 2(b) with results from tight binding model in accumulation region. (b) The same wavefunction penetration has been obtained for all the models using the pseudo oxide band structure model of Figure 3.

on the influence on capacitances (Figure 6), energy levels and waves (Figure 7). In this case a full meshing on K in reciprocal space is performed for the accurate computation of the inversion charge. In Figure 6, an oxide mass value of $0.45m_0$ has been used in the EMA model in order to amplify the small differences noticeable between the 30-k.p and EMA models after the ab-initio calibration. Smaller differences could be found with the fitted value of $1.7m_0$ obtained from ab-initio calculations. Also in this case the impact of strain on the valence bands has been analyzed and modeled in EMA using the analytical solution of the 6-k.p Bir-Pikus model at Γ [6]. Due to the reduced band splitting of the Γ valleys in inversion, the SL has a negligible impact on the inversion charge and has not been showed in the Figure.

III. Modeling of interfacial layers

The SiO_2/Si interface is modeled using a 5Å-thick interfacial layer region where the electro–chemical properties of the material are linearly varying. The variations of the band structure parameters used in the Shrodinger solver are also taken into account. Additionally 2D TCAD simulations have been performed using a commercial simulation package [7] to assess the predictions of the models implemented in TCAD tools (Figure 8(a)). The density gradient model included in the simulation tool provides the control over two fitting parameters γ_e

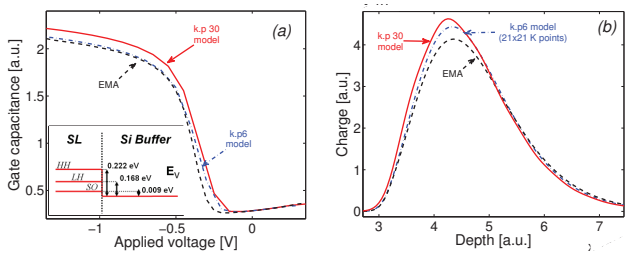

Figure 6: (a) C-V curves comparing a 3-band EMA model and a 30-k.p model (including a full meshing on K in reciprocal space) for holes in inversion on the device shown in Figure 2(b). Additionally, the inset shows the impact of strain in the layer on the valence band. (b) Comparison of inversion charges calculated for two different bias voltages on the same device at $V_G = -1.15V$.

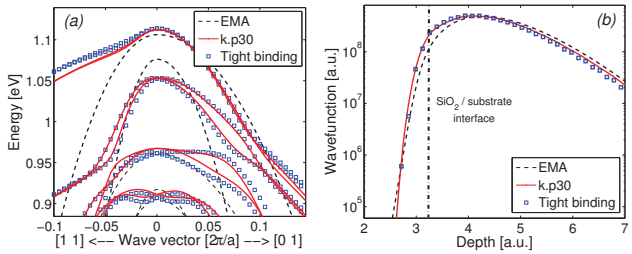

Figure 7: (a) Comparison between the band structures obtained with 30-k.p, 3-band EMA and sp3d5s* tight binding model in inversion region ($V_G = -1.15V$). (b) Wave function penetration in the oxide region obtained with the 3 models. Also in this case, to further illustrate the difference with EMA, $m_{ox} = 0.45m_0$ has been used leading to a smaller penetration in the oxide.

and γ_h, used for modulating the variation of electrons and holes Fermi levels, respectively. Figure 8(b) and 8(c) show how the variation of the IL thickness (ranging from 5Å to 10Å on Si [2]) is influencing both the capacitance and the inversion charge, affecting the threshold voltage of the device. It is worth mentioning that a simple variation of dielectric permittivity or oxide thickness is not sufficient to match the full CV curve for all the devices, since the model predictions will eventually fail in the depletion region.

Conclusion

In this paper, the impact of advanced band structure models and interfacial layers on electrical characteristics has been demonstrated. After a refined calibration on first principles simulations, computationally expensive tight binding and full band k.p models have been compared to EMA models in order to accurately extract the band structure parameters. Additionally, the effects of

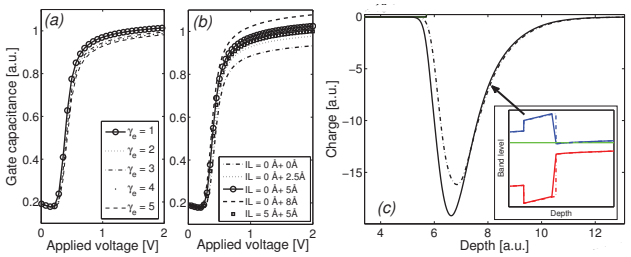

Figure 8: (a) TCAD simulation results on device shown in Figure 1(a) using the density gradient model both in accumulation and inversion regions. (b) 3-bands EMA simulation results on device (a), showing the capacitance variation in inversion when the IL thickness is changed. (c) The physical reason of the capacitance increase with IL is due to the higher penetration of the wavefunctions in the IL and in the oxide, consequently increasing the total inversion charge. The same effect can be seen in accumulation. The inset shows how the band diagram is modified after the inclusion of a 5Å-thick IL.

strain have been considered in all the implemented models and it has been showed how the impact of band splitting is playing a significant role on the accumulation charge. It has been proved that one has to take it into account to preserve model predictions in all device operating regions. Finally the effects of SiO_2/Si interface models have been studied comparing the results both to measurements and 2D TCAD simulations.

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