Student paper

Investigation of a MOSCAP Using NEGF

M. Karner, O. Baumgartner, M. Pourfath, M. Vasicek, and H. Kosina

Institute for Microelectronics, TU Vienna, Gußhausstraße 27–29,
1040 Wien, Austria, baumgartner@iue.tuwien.ac.at

Theoretical investigations on the MOS Capacitor, the heart of the MOSFET, have been early addressed by numerical simulations within a semi-classical treatment. Due to the strong impact of quantum mechanical effects for MOS inversion layers, quantization effects are taken into account by treating two-dimensional sub-band states [1]. For accumulation layers, this is highly problematic because besides the discrete states, there is a non negligible contribution of the continuum states. A more rigorous investigation by applying the non-equilibrium Green's functions (NEGF) formalism [2] does not suffer from this problem and directly yields the current. The influence of level broadening due to scattering process was modeled by means of an optical potential, which is discussed in detail. An analysis of the MOSCAP has been carried out using the non-equilibrium Green's function formalism. The gate and the bulk regions have been assumed to be in thermal equilibrium which implies a constant Fermi energy $\mathcal{E}_{\mathrm{FG}}$ and $\mathcal{E}_{\mathrm{FB}}$, respectively. The leakage current through the gate oxide, which separates the equilibrium regions, has been calculated assuming ballistic transport between the two reservoirs [3, 4]. The retarded and advanced Green's functions are determined by the equation

$$G^{\mathrm{R}}(\mathbf{r},\mathbf{r}',\mathcal{E}) = G^{\mathrm{A}\dagger}(\mathbf{r},\mathbf{r}',\mathcal{E}) = [\mathcal{E}I - H(\mathbf{r},\mathbf{r}',\mathcal{E}) - \Sigma^{\mathrm{R}}(\mathbf{r},\mathbf{r}',\mathcal{E})]^{-1},$$

where $H(\mathbf{r},\mathbf{r}',\mathcal{E})$ is the Hamiltonian of the system and $\Sigma^{\mathrm{R}}(\mathbf{r},\mathbf{r}',\mathcal{E})$ is the retarded self-energy. The optical potential, which follows from the carrier lifetime τ is added to the diagonal elements of the Hamiltonian: $H(\mathbf{r},\mathbf{r},\mathcal{E}) = H_0(\mathbf{r},\mathbf{r},\mathcal{E}) + \imath\hbar/(2\tau)$.
Within the equilibrium regions, the lesser Green's function is calculated as

$$G^{<}(\mathbf{r},\mathbf{r}',\mathcal{E}) = G^{\mathrm{R}}(\mathbf{r},\mathbf{r}',\mathcal{E}) f_{\mathrm{G,B}}(\mathcal{E})$$

with the occupation function $f_{\mathrm{G,B}}(\mathcal{E})$ of the gate and bulk, respectively. The lesser Green's function in the oxide is determined by

$$G^{<}(\mathbf{r},\mathbf{r}',\mathcal{E}) = G^{\mathrm{R}}(\mathbf{r},\mathbf{r}',\mathcal{E})\Sigma^{<}(\mathbf{r},\mathbf{r}',\mathcal{E})G^{\mathrm{A}}(\mathbf{r},\mathbf{r}',\mathcal{E}).$$

The lesser self energy of the left and right contact writes as $\Sigma^{<}_{\mathrm{G,B}}(\mathcal{E}) = \imath\Im\left\{\Sigma^{\mathrm{R}}_{\mathrm{G,B}}(\mathcal{E})\right\} f_{\mathrm{G,B}}(\mathcal{E})$. The electron density and the leakage current are given by the integrals

$$n(\mathbf{r}) = -2\imath \int G^{<}(\mathbf{r},\mathbf{r},\mathcal{E}) \frac{\mathrm{d}\mathcal{E}}{2\pi},$$
$$j(\mathbf{r}) = -\frac{\hbar q}{m^*} \int \left[(\nabla - \nabla')G^{<}\left(\mathbf{r},\mathbf{r}',\mathcal{E}\right)\right]\Big|_{\mathbf{r}'=\mathbf{r}} \frac{\mathrm{d}\mathcal{E}}{2\pi}.$$

A MOS capacitor (n$^+$-insulator-p$^+$) with a doping of $N_{\mathrm{D}} = 1 \times 10^{19}\,\mathrm{cm}^{-3}$, $N_{\mathrm{A}} = 5 \times 10^{17}\,\mathrm{cm}^{-3}$, and a dielectric thickness $t_{\mathrm{diel}} = 1.2\,\mathrm{nm}$ has been investigated. Fig. 1 shows the local density of states of the device under a gate bias of 1.2 V. The spectrum of the current is shown in Fig. 2. The peaks at the resonance energies which correspond to the quasi-bound states give the main contribution to the gate leakage current. Although the resonance width is strongly affected by the carrier lifetime, there is only a slight change in leakage current as depicted in Fig. 3. It is shown that the macroscopic quantities are only slightly affected by the optical potential(c.f. Fig. 3).
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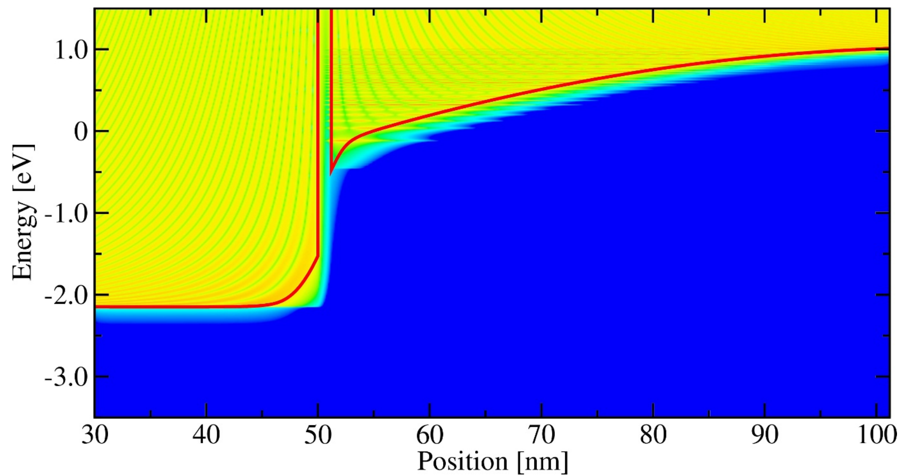

Figure 1: Self consistent band edge energy and the local density of states. It features quantum mechanical effects like the penetration of the wavefunctions into classically forbidden regions and reflections at the barrier. Furthermore, within the channel, the formation of quasi-bound states and the transition to the continuum states can be clearly seen.

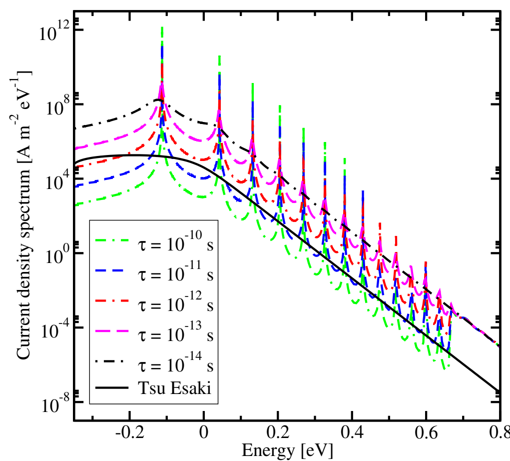

Figure 2: The Current spectra. The energetic broadening of the QBS due to the optical potential can be clearly seen.

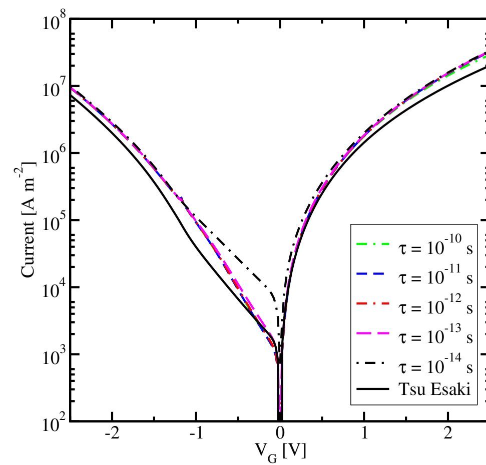

Figure 3: The leakage characteristic of the device. Although the optical potential yields a broadening of the resonance width, the current is nearly unaffected.

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