Numerical and semi-analytical analysis of modulation layer properties in ITO modulators.

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Abstract— **classical (numerical and semi-analytical) and quantum models for the effective charge accumulation/depletion layer depth in a metal-dielectric-Indium Tin Oxide modulator are compared. Both are shown to give results of the order of 0.1 nm, justifying modeling the layer in optical simulations as a two-dimensional object, for which the predictions of both models are very similar.**

Keywords—ITO, modulator, numerical modeling.

I. Introduction

Metal-insulator-Indium Tin Oxide (ITO) modulators are promising for a number of applications due to uniquely strong modulation potential [1][2], and have been studied by a number of groups both experimentally and theoretically/numerically. In numerical modelling, ITO is treated as a highly *n*-doped (N_D^+ ~10^{19}-19^{21} cm^{-3}) semiconductor. The accumulation or depletion layer (which is the active layer of the modulator) is sometimes represented in models as a spatially homogeneous layer at the semiconductor-dielectric interface [3], with modulation voltage dependent complex dielectric permittivity, but the layer thickness *l* used by various authors varies widely from <1 nm [2] to 5 nm [1]. Estimating this depth usually involves commercial [2] or in-house [3] numerical models with no or limited analytical progress. All models so far have been purely classical, which is somewhat tenuous as the order of magnitude of *l* is ~ 1 nm. Here, I attempt to gain more analytical insight into the *l* value and its dependence on parameters, compare the results of classical and (simplified) quantum mechanical approaches, and discuss the implications for optical modelling of ITO modulators.

II. The structure.

The part of the structure relevant to the model consists of a metal contact (assumed ideal ohmic), a dielectric/insulator layer with a thickness l_i of the order of a few nanometres, and the ITO layer (thickness >> *l*) as in [2].
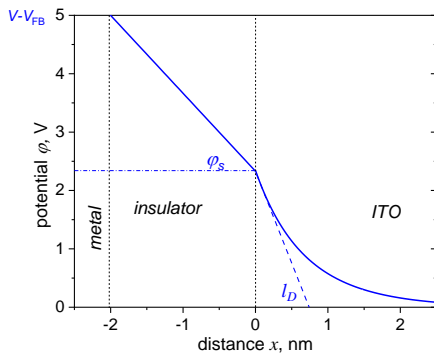

Fig. 1. Typical structure and potential distribution

III. The classical model

The classical approach to determining the carrier distribution within the accumulation/depletion layer in the ITO requires solving one-dimensional Poisson's equation $d^2\varphi/dx^2 = e(n(\varphi) - N_D^+)/(\varepsilon_{rs}\varepsilon_0)$ together with the continuity of the absolute position of the Fermi level inside the ITO which determines the carrier density $n(\varphi(x))$ inside the layer. The boundary conditions for the potential $\varphi(x)$ are in the bulk of the ITO and

$$\varphi_s - \frac{\varepsilon_{rs}}{\varepsilon_{ri}} \frac{d\varphi}{dx}\bigg|_{x=0+} l_i = V_g - V_{FB} \qquad (1)$$

at the insulator/ITO interface $x=0$, where $\varphi_s = \varphi|_{x=0+}$, ε_{rs}, ε_{ri} are the dielectric constants of ITO and the insulator, respectively, V_g is the voltage applied to the gate (metal contact), and V_{FB} is the built-in "flat-band voltage" of the structure, estimated from the difference between the work functions of the materials involved. Adapting the textbook approach of [4] to the case of degenerate statistics, the problem is reduced to a first-order differential equation allowing the electric field to be calculated formally as the function of $\varphi(x)$:

$$\frac{d\varphi}{dx} = -\sqrt{2\frac{eN_D^+k_BT}{\varepsilon_s}}F\left(\frac{e\varphi}{k_BT}\right) \qquad (2)$$

The function F is defined by the form of $n(\varphi(x))$. In the case of *full* degeneracy, accurate for accumulation and moderate depletion, it can be calculated analytically as

$$F^2(y) = 0.4\mu\left[\left(1 + y/\mu\right)^{5/2} - 1\right] - y; \quad \mu = E_F/(k_BT) \qquad (3)$$

where in this case the Fermi level in the bulk of the ITO is found from the standard formula $E_F \approx \hbar^2\left(3\pi^2 N_D^+\right)^{2/3}/(2m_e)$. Applying (2)-(3) at *x*=0 and combining it with (1) gives a transcendental equation from which both $\varphi_s = \varphi|_{x=0}$ and $d\varphi/dx|_{x=0+}$ can be found. This provides the boundary condition with which the full $\varphi(x)$ profile (Fig.1) is easily calculated from (2), and also gives one estimate for the effective depth of the layer – the generalised Debye radius:

$$l_D = [\varphi |d\varphi/dx|^{-1}]|_{x=0+} \qquad (4)$$

Near the flat-band condition ($V \approx V_{FB}$), a simple analytical estimate for $l_{Dd} = l_D(0)$ can be found from (3-4):

$$l_{Dd} \approx \pi^{2/3}\frac{\hbar}{e}\sqrt{\frac{\varepsilon_{rs}\varepsilon_0}{m_e}}\left(3N_D^+\right)^{-\frac{1}{6}} \qquad (5)$$

With parameter values from [1]-[2], this gives around 0.75 nm; note also the very weak dependence on the carrier density. The full calculated $l_D = l_D(V-V_{FB})$ is shown as a dashed line in Fig.2 showing good agreement with the estimate (5)

and a decrease of l_D with voltage. An alternative estimate for the layer depth can be obtained by weighting the carrier density distribution [2] i.e. numerically integrating (2), calculating $n(\varphi(x)) = N_D^+ \left(1 + \varphi(x)/E_F\right)^{3/2}$ and defining

$$l_a = \left(n(\varphi|_{x=0}) - N_D^+\right)^{-1} \int_0^\infty \left(n(\varphi(x)) - N_D^+\right) dx \qquad (6)$$

This estimate is shown in Fig.2 as a solid line. The values are quite close to those of l_D calculated from (4), implying that the potential distribution is not too far from a simple exponential.
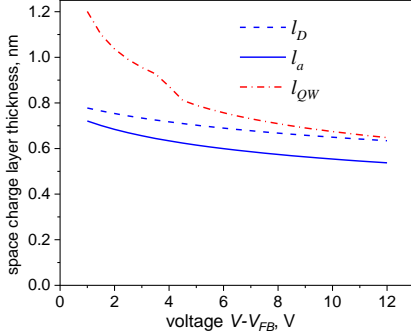

Fig.2. Effective depth of the space charge layer as function of voltage. l_i=5 nm; m_e=0.35m_0; ε_{rs}=9.4, ε_{ri}=25, $N_D^+ = 3 \times 10^{20}$ cm^{-3}

IV. THE SIMPLIFIED QUANTUM ESTIMATE.

Since the results confirm the nanometre order of the length scales involved, it is of interest to estimate the possible extent of quantum effects in the charge layer profile. The opposite extreme from the purely classical model of the previous section is a *single-particle* quantum model. In the most accurate form, this would involve a Schrödinger-Poisson solver. In a simplified version used here, we use the prediction that the potential profile is not too far from exponential, and approximate the potential profile associated with the accumulation layer with a single-sided exponential well:

$$U(x)|_{x>0} = -e\varphi(x); \quad \varphi(x) = \varphi_s \exp\left(-x/l_{QW}\right) > 0 \qquad (7)$$

The characteristic space charge layer depth l_{QW} and the surface potential $\varphi_s = \varphi|_{x=0}$ are the parameters to be determined from analysis. The electrons are then divided into two populations: free electrons with the volume density of N_D^+, compensated by the ionised donors, and quantum confined electrons within the well which create the layer charge. From Poisson's equation, the electric field at the interface is proportional to the two-dimensional (2D) density of confined electrons. In the approximation of full degeneracy and using (7), a quantum mechanical (QM) equivalent of (2) for x=0 is

$$\frac{\varphi_s}{l_{QW}} = \frac{e}{\varepsilon_s} \frac{m_e}{\pi\hbar^2} \sum_m \left|\mathrm{E}_m(\varphi_s, l_{QW})\right| \qquad (8)$$

, where $\mathrm{E}_m(\varphi_s, l_{QW}) < 0$ are the energies of the bound levels in the QW, found by solving Schrödinger's equation for the profile (7). Combining this with the QM equivalent of (1)

$$\varphi_s \left(1 + \varepsilon_{rs} l_i / (\varepsilon_{ri} l_{QW})\right) = V_g - V_{FB} \qquad (9)$$

one obtains a system of two transcendental equations, from which l_{QW} and φ_s can be found. The value of l_{QW} as function of voltage is shown in Fig.2 alongside the classical estimates. The value is only slightly greater than l_D and l_a and shows

similar qualitative tendencies. A more accurate, many-body, result is likely to come even closer to the classical predictions.

V. IMPLICATIONS FOR OPTICAL MODELING.

In the optical models, the complex dielectric permittivity of ITO is approximated by the Drude formula and thus is proportional to the carrier density. Since both the classical calculation and the quantum estimate give the values of l of the order of 1 nm, substantially narrower than the mode of any waveguide, whether dielectric or plasmonic, one can confidently assume that it is only the *two-dimensional* electron density N_{2D}, rather the spatial distribution $n(x)$, that is important in an optical model. This is equivalent to treating the layer as a thin rectangular one as proposed in [3]. N_{2D} can be evaluated as

$$N_{2D} = (\varepsilon_{rs}\varepsilon_0/e) \left.\left|\mathrm{d}\varphi/\mathrm{d}x\right|\right|_{x=0+} \qquad (10)$$

in both the classical and quantum models. The results are shown in Fig.3 and are remarkably similar, particularly if the insulator thickness l_i is at least a few times greater than l (lower curves; this is the case in many practical designs, e.g. in [2]). Indeed in this case, the voltage drop in the entire system is dominated by the insulator rather than the ITO, so N_{2D} is estimated in the first approximation as just $N_{2D} \approx \varepsilon_{ri}\varepsilon_0 \left(V_g - V_{FB}\right)/(el_i)$, regardless of the ITO properties and the model used to describe them.
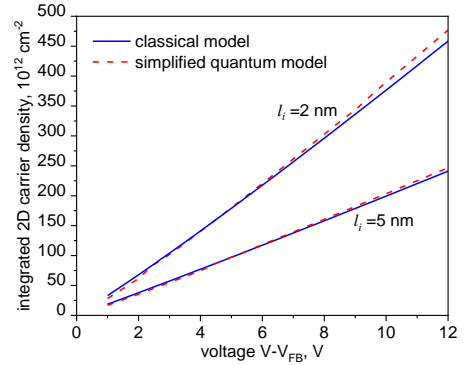

Fig. 3. Integrated 2D carrier density in the space charge layer as function of applied voltage for two values of the insulator spacer layer thickness.

With thinner insulator layers ($l_i \sim l$), more accurate analysis is required (upper curves in Fig. 3); a semi-analytical classical model as discussed above is arguably the simplest and sufficiently accurate for that purpose.

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