An analytical expression of electric potential and field of organic thin film transistors

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Abstract. The two-dimensional electric potential and field of an organic thin-film transistor (OTFT) is derived by conformal mapping using the Schwarz-Christoffel-transformation of the Poisson equation. In this paper we compare this analytical closed-form solution to field simulation results from Silvaco TCAD. Inter alia the potential close to the surface is calculated and we found excellent accordance to the numerical simulations and thus proofed its usability for charge transport calculations. Thus, it is used for calculation of the drain-source-current in the channel.

1. Introduction
The growing development of electronics and its wide use in all kinds of industries has led to the need of decreasing cost per function and area respectively of electronic devices. Until now, more integration of devices, i.e. growing number of transistors in a defined area, integration of functionalities etc., results in a reduction of costs. Another mean to minimize chip costs is organic electronics. The use of low cost fabrication like spin-coating or printing leads to very cheap devices. Still, the development of electronics and also organic electronics would not have been possible without robust CAD and simulation tools. These tools require accurate models to describe a single device and whole circuits made up of them. These models should be both accurate and fast in terms of computing time. Therefore, analytical equations are needed as only these fulfill both claims.

Because OTFTs follow other basic physical principles than inorganic semiconductors, models for circuit simulators must be developed which take the physics of the organic material into account. In order to obtain models that rely on these organic properties information of physical parameters within the channel have to be acquired. We therefore started with a simulation of the electric field and potential of an OTFT and compared the results to an analytical expression obtained by the mean of conformal mapping for the potential within the channel.

2. Conformal Mapping
As it is difficult to solve the Poisson-equation in a two-dimensional area, conformal mapping is used to transfer the two-dimensional channel region of the OTFT into a one-dimensional. In this geometry the solution can be obtained easily. The idea behind conformal mapping is that the problem with a geometry that is rather difficult to solve may be mapped into a problem with simple geometry or with a geometry where the solution is known. The channel region with
The OTFT structure in z-plane is described by a rectangle with electrode source=BC, drain=AD and AB corresponding to the gate-dielectric-channel capacitor plate below the dielectric.

Figure 1. OTFT Structure before and after conformal mapping

its polygonal boundaries, i.e. source, drain and gate electrode, can be mapped into an upper half-plane by the use of the Schwartz-Christoffel transformation [1] [2].

We started with an OTFT geometry shown in figure 1(a) with real axis \( x \) and \( y \) and the channel region with source electrode BC, drain electrode AD and AB corresponding to the gate-dielectric-channel capacitor plate below the dielectric [2]. Applying conformal mapping figure 1(a) is transformed to figure 1(b) with real axis \( u \) and imaginary axis \( v \). The channel region within the rectangle, where the Poisson equation will be applied, is mapped into the upper half-plane in figure 1(b). Here the unit length \( L = 1 \) of the channel is chosen. The Schwarz-Christoffel differential equation for transformation of the \( w \)-plane (figure 1(b)) to the \( z \)-plane (figure 1(a))

\[
\frac{dz}{dw} = S(w - 1)^{-\frac{1}{2}}(w + 1)^{-\frac{1}{2}}
\]

is integrated to obtain the transformation from \( w \)- to \( z \)-plane:

\[
z = S \int_0^t \frac{dt}{\sqrt{(w - 1)(w + 1)}} + K
\]

The integration constant \( K = 0 \) is obtained from the assumption, that both coordinate systems \( w = u + iv \) und \( z = x + iy \) have the same origin, so \( w = z = 0 \). The pre-factor \( S \) is derived from the mapping theory and equals \( L/\pi \), resulting in the final transformation

\[
z = f(w) = 2 \frac{L}{\pi} \ln\left(\frac{\sqrt{w - 1}\sqrt{w + 1}}{\sqrt{2}}\right)
\]

The reverse transformation follows this equation:

\[
w = f^{-1}(z) = \frac{e^{\frac{\pi}{L}z} + e^{-\frac{\pi}{L}z}}{2} = \cosh\left(\frac{\pi z}{L}\right)
\]

The separation of real part \( u \) and imaginary part \( v \) leads to:
\begin{equation}
 u = \frac{e^{\frac{\pi x}{L}} \cos(\frac{\pi y}{L}) + i \sin(\frac{\pi y}{L})}{2} \tag{5}
\end{equation}

\begin{equation}
 v = \frac{e^{-i\pi x} \cos(\frac{\pi y}{L}) + i \sin(\frac{\pi y}{L})}{2} \tag{6}
\end{equation}

3. Calculation of electric potential and field

The distribution of the electric potential in the channel of an OTFT can be calculated from the Poisson equation

\begin{equation}
 \Delta \Phi(x, y) = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = -\frac{\rho}{\epsilon_r \epsilon_0} \tag{7}
\end{equation}

where \( \rho \) denotes the charge density, \( \epsilon_r \) and \( \epsilon_0 \) are the relative and vacuum permittivity, respectively. Organic semiconductors usually are unipolar. As they are lightly doped \( \rho \) is very small and can be set to zero [3]. Thus, \( \rho = 0 \) and the Poisson equation becomes the Laplace equation

\begin{equation}
 \Delta \Phi(x, y) = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = 0 \tag{8}
\end{equation}

As mentioned in the section before, the Poisson and the Laplace equation respectively are mapped to the upper-half plane for computation with less complexity. Considering an upper-half plane with \( u \) as real axis and \( v \) as imaginary axis, the boundary condition is \( \phi(u, 0) = P(u) \). The solution of the Laplace equation in that plane is [1]

\begin{equation}
 \Phi(u, v) = v \int_{-\infty}^{\infty} \frac{P(t)}{(u-t)^2 + v^2} dt \tag{9}
\end{equation}

Assuming the source S to be the boundary for \(-\infty < u < -1\), the area below the dielectric for \(-1 \leq u \leq 1\), and drain D for \(1 < u < \infty\), with boundary conditions \( \phi_s, \phi_{\text{diel}}, \) and \( \phi_d \), (9) results in

\begin{equation}
 \Phi(u, v) = \frac{\phi_d + \phi_s}{2} + \frac{\phi_{\text{diel}} - \phi_d}{\pi} \cdot \arctan\left(\frac{u + 1}{v}\right) \\
+ \frac{\phi_s - \phi_{\text{diel}}}{\pi} \cdot \arctan\left(\frac{u - 1}{v}\right) \tag{10}
\end{equation}

Taking \( u \) and \( v \) of (5) and (6) into the solution of the Laplace equation (10), the channel electric potential distribution in the original \( z \)-plane (figure 2) is obtained:

\begin{equation}
 \Phi(x, y) = \frac{\phi_d + \phi_s}{2} \\
+ \frac{\phi_{\text{diel}} - \phi_d}{\pi} \cdot \arctan\left(\frac{\cos\left(\frac{\pi y}{L}\right) \cosh\left(\frac{\pi x}{L}\right) + 1}{\sin\left(\frac{\pi y}{L}\right) \cdot \sinh\left(\frac{\pi x}{L}\right)}\right) \\
+ \frac{\phi_s - \phi_{\text{diel}}}{\pi} \cdot \arctan\left(\frac{\cos\left(\frac{\pi y}{L}\right) \cosh\left(\frac{\pi x}{L}\right) - 1}{\sin\left(\frac{\pi y}{L}\right) \cdot \sinh\left(\frac{\pi x}{L}\right)}\right) \tag{11}
\end{equation}

The surface potential \( \Phi_{\text{surf}} \) is obtained for \( y = 0 \). The electric field \( \vec{E} \) is calculated from
Replacing again $u$ and $v$ of (5) and (6) into (12) results in the electric field distribution in the channel. The total semiconductor surface charge is obtained from Gauss Law

$$Q_{surf} = -\varepsilon_{vacuum} E_y.$$  \hfill (13)

In our model this is the charge responsible for the current conduction. The current $I_{DS}$ from source to drain in the channel is calculated by

$$I_{DS} \propto \int_0^L Q_{surf} E_x dx \propto \int_0^L E_x E_y dx. \hfill (14)$$

4. Comparison to TCAD results

We compared the analytically obtained solution of the Laplace equation with the numerical result of Silvaco TCAD [4]. The device structure has been build according to figure 2, using gold as electrode material for source, drain and below the dielectric in order to emulate the potential at the gate-dielectric-channel capacitor and an organic semiconductor already implemented in the simulation environment of Silvaco TCAD in the channel region. The size of the geometry is chosen in such a way that the simulation results are comparable to the analytical solution for unit length $L = 1$.

TCAD solves coupled Poisson and drift diffusion equations

$$\nabla \cdot [\varepsilon \nabla \Phi] = -q \left( p - n + N_D^+ - N_A^+ + p_{At} \right) \hfill (15)$$

$$\nabla \cdot J_n = q \left( R - G \right) \hfill (16)$$

$$\nabla J_p = -q \left( R - G \right) \hfill (17)$$

$$J_n = -q\mu_n \nabla \Phi + qD_n \nabla n \hfill (18)$$

$$J_p = -q\mu_p \nabla \Phi - qD_p \nabla p \hfill (19)$$

The electric potential for a device as in figure 2 for the boundary condition values $\phi_s = 0$, $\phi_{d\text{iel}} = 2$, and $\phi_d = 3$ is shown in figure 3 for the calculation of the potential. A cut parallel to the $x$-axis and perpendicular to the $y$-axis, i.e. parallel to the dielectric, at $y \to 0$ plots the potential $\phi_{surf}$ close to the surface and is shown in figure 4(a). The right $y$-axis shows the error, i.e. the
difference $\Phi_{surf,simulated} - \Phi_{surf,calculated}$ between the simulated and calculated potential close to the surface. It can be clearly seen that our analytical solution fits very precisely to the numerical solution of the Laplace equation. Thus, our analytical expression for the electric potential and field can be used to simulate charge transport in organic semiconductors more accurately and will lead to more precise models for circuit simulation. We have taken the calculated current in the channel of equation (14) to obtain a transfer curve in figure 4(b). In this semilogarithmic plot it can be seen that the current follows the well-known transfer-shape.

5. Conclusion
We have derived an analytical closed-form solution of the Poisson equation to obtain the electric potential and field in the channel of an OTFT. We transformed the rather hard to solve geometry, i.e. the rectangular shaped OTFT channel, to an upper half plane by conformal mapping where the Poisson equation can be solved easily. The obtained analytical expression for the electric potential and field are compared to numerical solutions by Silvaco TCAD and show excellent agreement.

![Graphs showing comparison of simulated and calculated results.](image)

Figure 4. surface potential and resultant transfer curve of the current

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