Numerical evaluation of the dipole-scattering model for the metal-insulator transition in gated high mobility Silicon inversion layers

T. Hörmann and G. Brunthaler
Johannes Kepler Universität, Linz, A-4040, Austria
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The dipole trap model is able to explain the main properties of the apparent metal-to-insulator transition in gated high mobility Si-inversion layers. Our numerical calculations are compared with previous analytical ones and the assumptions of the model are discussed carefully. In general we find a similar behavior but include further details in the calculation. The calculated strong density dependence of the resistivity is not yet in full agreement with the experiment.

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I. INTRODUCTION

Since it’s discovery in 1995, the metal-insulator transition in two dimensions (2D) was investigated carefully, as it’s finding is in apparent contradiction to the scaling theory of localization. According to the latter, in the limit of zero temperature, a metallic state exists only in three dimensions, but in two dimensions disorder should always be strong enough in order to lead to an insulating state. Nevertheless, high-mobility n-type silicon inversion layers showed for high electron densities a strong decrease of resistivity $\rho$ towards temperatures below a few Kelvin, manifesting the metallic region, and a strong exponential increase of the $\rho$ for low densities demonstrating the insulating regime. A very similar behavior was observed in many other semiconducting material systems at low temperatures.

After the unexpected finding, several models were suggested in order to explain the metallic behavior in 2D. The most important ones are i) temperature-dependent screening, ii) quantum corrections in the diffusive regime, iii) quantum corrections in the ballistic regime, and iv) scattering of electrons according to the dipole trap model. As there are argumentations for all that different models in the literature, we do not want to repeat them here in detail. A clear decision for one of the suggestions could not been drawn yet and further work on the models has to be carried out.

The dipole trap model was introduced by Altshuler and Maslov (AM) especially for Si-MOS structures, as it is known that the misfit at the silicon/silicon-oxide interface produces charged defect states in the thermally grown oxide layers. AM could show that a hole trap level at energy $E_t$ which is either filled or empty, depending on its position relative to the Fermi energy $E_F$, can lead to a critical behavior in electron scattering if $E_t$ and $E_F$ are degenerate. This dipole trap model can explain the main properties of the metal-insulator transitions in gated Si-MOS structures.

In this work, we present numerical calculations of the temperature and density dependent resistivity due to electronic scattering in the dipole trap model. With these calculations we are able to checking the analytical calculations with its approximations. Due to the numerical procedure, we can include further details and investigate their influence.

For the analytical calculations AM made a number of assumptions. These are: a) the trap states possess a 4-like distribution in energy, a2) the spatial distribution in the oxide is homogeneous, a3) the occupied states are positively charged and lead to scattering (hole trap), a4) a charged trap state is effectively screened by the 2D electrons so that the resulting electrostatic potential can be described by the trap charge and an apparent mirror charge with opposite sign on the other side of the interface, a5) the scattering efficiency of the 2D electrons is described by a dipole field of the trap charge and it’s mirror charge, a6) a parabolic saddle point approximation for the total potential of the trap states was used in order to perform analytical calculations, a7) the energy of the trap state $E_t$ is fixed relative to the quantization energy $E_0$ of the 2D ground state inside the inversion potential, and a8) the Fermi energy $E_F$ in the 2D layer is either independent of or is the same as in the 3D substrate.

In contrast to AM, our calculations were performed numerically, so that several limitations of their calculations could be dropped. Our improvements concern i1) the detailed spacial dependence of the electrostatic potential is taken into account instead of the parabolic saddle point approximation, i2) the energy of the trap state $E_t$ is fixed relative to the conduction band edge $E_{CB}$. As a result of our calculations, we find a similar behavior of the calculated resistivity as AM and we calculate in addition the density dependence of the resistivity.

According to the restricted space in the original AM work, some of the used equations were not derived there. We will discuss these equation and considerations in detail in the main part. For better readability of our paper, some details were put into appendices. Please note that
we will use SI units throughout this work.

II. MODEL CONSIDERATIONS AND NUMERICAL CALCULATIONS

The misfit at the Si/SiO\textsubscript{2} interface layer leads to different kinds of defects and trap states\textsuperscript{13,14,15,17}. In the considered AM model it is assumed that a relative large number of hole trap states exists. If such a trap state captures a hole, it is positively charged, otherwise it is neutral. In Fig. 1 the trap state is depicted schematically.

![FIG. 1: Schematic representation of the trap state together with the 2D electron system (2DES). For $E_t > E_F$ the trap state is positively charged and scatters electrons in the 2D layer whereas for $E_t < E_F$ the trap is neutral, i.e. it is occupied with an electron and does not act as a scattering center. Note that the main recharging effect comes from the energetic position $E_t$ of the trap state. It varies strongly with the applied gate voltage $V_g$, whereas the Fermi-energy $E_F$ shows only small variations with changing electron density on the same scale.](image)

As described in the introduction, it is further assumed that a1) all trap states exist at the same energy $E_{t0}$ if no external field is applied and posses a2) a spatially homogeneous density distribution in the oxide layer. But a potential gradient due to an applied gate voltage $V_g$ causes a linear increase of the trap energy position $E_t = E_{t0} + e V_g z / d$, where $z$ is the distance from the Si/SiO\textsubscript{2} interface ($z < 0$) and $d$ is the distance between gate electrode and that interface (i.e. the thickness of the oxide layer).

For the electrostatic potential inside the oxide layer, also the screening effects of the inversion layer have to be taken into account. For 2D electrons in a Si-(001) layer, the screening radius is equal to $a_B/4$. If the trap distance from the interface $|z|$ exceeds the screening radius, the in-plane components of the electrostatic field caused by the charged trap will effectively be screened. In that case, the electric field and the potential in the oxide can be described by the trap charge and an apparent mirror charge with opposite sign on the other side of the interface (assumption a4). The potential of the charged trap state caused by the image charge is $\Phi = e / (2 \cdot 4\pi \varepsilon_0 \varepsilon_{\text{ox}} z)$ in SI units with $\varepsilon_0 = 8.854 \times 10^{-12}$ Fm$^{-1}$ and $\varepsilon_{\text{ox}} \approx 3.9$, the relative dielectric constant of the oxide. Thus the total energy of the charged trap state can be given as

$$E_t(z) = E_{t0} + e V_g z / d + e^2 / 8\pi \varepsilon_0 \varepsilon_{\text{ox}} z$$

for $z < 0$.\textsuperscript{11}

The last term in Eq. 1 leads to a down bending of the energetic position towards the interface and causes a maximum in the total trap energy $E_t(z)$ as shown in Fig. 2.

![FIG. 2: Schematic representation of energies in the dipole trap model. The dashed blue line on the left represents the trap energy without, the full blue line with mirror charge potential. Note that the distance scale on the left and right hand side of the interface is chosen differently in order to increase visibility.](image)

The trap charge together with its mirror charge form a dipole perpendicular to the interface plane. Thus, for distances larger than $2|z|$, the scattering potential experienced by the 2D electrons can be described by a dipole field which falls off with $1/r^3$ (assumption a5). This is in agreement with the long range field of a screened Coulomb potential in two dimensions and leads to a consistent description. AM have calculated the classical scattering cross section for momentum relaxation $\sigma_m(E, z)$ for such a dipole field for electrons with kinetic energy $E$ as

$$\sigma_m(E, z) = 2.74 (e^2 z^2 / 8\pi \varepsilon_0 e^* E)^{1/3}$$

with $e^* = (\varepsilon_{\text{ox}} + \varepsilon_{\text{Si}})/2 \approx 7.9$, the effective dielectric constant for the 2D electron system (2DES).

Whether a trap state is charged or not, depends on its energetical position relative to the Fermi energy $E_F$ (assuming thermal equilibrium for the occupation). The occupation function corresponds to a modified Fermi-Dirac distribution, where the degeneracy of empty and filled states is taken into account. AM have assumed that the (positively) charged trap state can have either spin up or down and is thus doubly degenerate, while the neutral state has no degree of freedom and is not degenerate. From that the probability of a trap state to be charged follows as

$$p^+(z) = \frac{1}{1 + \frac{1}{2} \exp \left( \frac{E_F - E_t(z)}{kT} \right)}$$

with $k$ the Boltzmann constant.
For the occupation of the trap states only the relative position of the trap energy \(E_t(z)\) to the Fermi energy \(E_F\) is important. But the difference \(E_F - E_t(z)\) can not be derived directly – it has to be calculated from the two individual energies which depend on different variables. According to Eq. 4 the \(z\)-dependence of the trap energy can be calculated, but one has to fix it’s zero-position \(E_0\). AM have assumed (a7) a fixedenergetical distance of the trap state relative to the quantization energy \(E_0\) of the electronic ground state in the (nearly triangular) inversion potential. But \(E_0\) depends on the strength and shape of the inversion potential and via electron-electron interaction on the 2D electron density \(n_s\). Thus it seems not realistic that the energy of the trap state is fixed relative to \(E_0\), but rather that it is fixed relative to the energetic position of the conduction band edge \(E_{CB}\) (which is our improvement i2).

Equation 4 can be used as given, by noting that the energy is defined relative to the conduction band edge \(E_{CB}\). On the other hand the ground state energy \(E_0\) has to be calculated for the inversion potential, which itself depends on \(n_s\) and the depletion charge \(N^-\) and by including the electron-electron interaction14. As \(E_F - E_0\) follows from the electron density \(n_s\), together with \(E_0\) one gets the position of \(E_F\) relative to the conduction band edge and the difference \(E_F - E_t(z)\) can be used for \(p^+(z)\) in Eq. 5.

In the Drude-Boltzmann approximation, the electrical resistivity \(\rho\), equal to the inverse conductivity \(\sigma\)

\[
\rho = \frac{1}{\sigma} = \frac{m^*}{ne^2} \frac{1}{\tau},
\]

follows by calculating the effective transport scattering time \(\tau\). The detailed calculation is performed in Appendix A.

As a result one gets that

\[
\frac{1}{\tau} = N_{\text{eff}}^+ v(\bar{E}) \sigma_m(\bar{E}, z_m),
\]

can be expressed by the effective values \(N_{\text{eff}}^+\) for the number of charged trap states per area, \(v(\bar{E})\) the electron velocity, \(\sigma_m(\bar{E}, z_m)\) the scattering cross section, and the average electron energy \(\bar{E}\) as given in Appendix A. These effective values depend on all the important variables of the systems, i.e. on \(T\), \(V_g\) and so on. By inserting Eq. 5 into Eq. 4 one gets already the dependence of the resistivity \(\rho\) on the different parameters

\[
\rho = \frac{m^*}{ne^2} N_{\text{eff}}^+ v(\bar{E}) \sigma_m(\bar{E}, z_m),
\]

and we have verified equation Eq. 7 in Ref. 12.

From here our treatment of the subject is quite different from that of AM. They have evaluated Eq. 4 analytically whereas we perform the calculation of it numerically. But in order to be able to solve Eq. 4 AM have used a parabolic (saddle-point) approximation for the \(z\)-dependence of the trap energy (assumption a6).

The analytical expression of AM (Eq. 9) contains a temperature independent prefactor \(\rho_0\) and a temperature dependent scaling function \(R(V_g, T)\). For their case (A) of the temperature dependence of \(E_F\), they get a critical behavior with \(R(T)\) increasing for \(V_g > V_g^c\) and decreasing for \(V_g < V_g^c\) (see Fig. 1 in Ref. 12), similar to what is observed experimentally. For their case (B), \(R(T)\) is always increasing with temperature and no critical behavior comes out.

In our numerical evaluation of Eq. 4 we use the exact dependence of \(E_t(z)\) as given by Eq. 4 (our improvement i2). The numerical treatment prevents errors due to the parabolic approximation, but enables us also to include further details, which also cannot be solved analytically.

AM have calculated the temperature dependence of the resistivity in close vicinity of the critical density where the behavior changes from metallic to insulating behavior. We have calculated also the direct density dependence over a larger range for different temperatures.

Fig. 3 shows how the effective number of charge trap states \(N_{\text{eff}}^+\) depends on \(n_s\).

![Figure 3: Effective number of charged trap states per area \(N_{\text{eff}}^+\) vs. electron density (i.e. varying gate voltage) at temperatures of \(T = 1, 3,\) and \(5\) K.](image)

As can be seen there is a very strong variation above \(n_s \approx 1.5 \times 10^{11} \text{ cm}^{-2}\), where the maximum of the trap energy \(E_t(z)\) is just degenerate with \(E_F\). This strong variation comes from the fact that as soon as the maximum of \(E_t(z)\) is below \(E_F\) only an exponentially small number of traps is still excited (i.e. charged) and the scattering efficiency decreases accordingly. As \(\rho\) is nearly proportional to \(N_{\text{eff}}^+\) such strong variations have not been observed experimentally. This discrepancy to the experiment can possibly be explained that in real 2D Si-MOS structures either the trap states do not have a \(\delta\)-like distribution in energy or that in addition other scattering sources exist.
III. CONCLUSIONS

We have shown that the numerical calculations of the temperature dependent resistivity give similar results as the analytical methods by AM. The strong density dependence of \( N^\pm \) and thus of \( \rho \) which follows from the calculation is not in agreement with experimental findings. In order to possibly resolve this discrepancy further calculations should be performed within the dipole trap model. The numerical procedure allows incorporation of further effects and realistic assumption like energetical broadening of the trap level, special spatial distributions of the defects, and detailed screening dependence.

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APPENDIX A: TRANSPORT EQUATIONS

The effective transport scattering time \( \tau \) in the Drude-Boltzmann approximation follows from

\[
\bar{\tau} = \frac{\int dE \tau(E) \frac{\partial f}{\partial E}}{\int dE \frac{\partial f}{\partial E}},
\]

(A1)

with \( \tau(E) \) being the energy dependent scattering time and \( \frac{\partial f}{\partial E} \) the first derivative of the Fermi-Dirac distribution function \( f \).

The transport scattering time \( \tau(E) \) has to be calculated over the individual scattering rates

\[
1/\tau(E) = \int_0^d dz N_+^z(z) v(E) \sigma_m(E, z)
\]

(A2)

with the density of charged traps \( N_+^z(z) = N_{G3} P_+(z) \), \( N_{G3} \) the spatially constant density of existing trap states (both being three dimensional volume densities) and \( v(E) \) the electron velocity.

By inserting the all expressions into Eq. A2 one gets

\[
1/\tau(E) = c' N_{eff}^{+} \frac{2/3}{m^*} E^{1/6}
\]

(A3)

with the prefactor \( c' = 2.74(e^2/8\pi\varepsilon_0\varepsilon_*)^{1/3} \sqrt{2/m^*} \), an effective number of positive trap states per area \( N_{eff}^+ = N_{G3} (\Delta z)^{eff} \), the effective width of positive charge layer \( (\Delta z)^{eff} = \int dz p_+(z)(z/z_m)^{2/3} \) and the position \( z_m = \sqrt{ed/8\pi\varepsilon_0\varepsilon_\alpha V_0} \) of the energetical maximum of the trap energy.

By inserting Eq. A3 into Eq. A1 one gets

\[
\bar{\tau} \propto 1/E_F \int_0^\infty dE E^{5/6} \frac{\partial f}{\partial E}.
\]

(A4)

Further an effective energy \( \bar{E} \) can be defined so that formally Eq. A3 can be preserved for the effective \( \bar{\tau} \), i.e. \( 1/\bar{\tau} = c' N_{eff}^{+} \frac{2/3}{m^*} \bar{E}^{1/6} \). A simple calculation gives

\[
\bar{E} = E_F \left[ \int_0^\infty dE \left( \frac{E}{E_F} \right)^{5/6} \frac{\partial f}{\partial E} \right]^{-6}.
\]

(A5)

By further replacing the first derivative of the Fermi-Dirac function by the identity \( \frac{\partial f}{\partial E} = - f(1-f) = - (4kT \cosh^2((E-E_F)/2kT))^{-1} \) one obtains the same expression as Eq. 8 in Ref. 12

With these relations, the resistivity can exactly be written in terms of the effective energy \( \bar{E} \) as

\[
\rho = \frac{m^*}{ne^2} N_{eff}^+ \bar{E} \sigma_m(\bar{E}, z_m),
\]

(A6)

which corresponds to Eq. 7 in Ref. 12 but the individual terms are rewritten according to our definitions above. A comparison with Eq. 4 gives exactly

\[
1/\bar{\tau} = N_{eff}^+ \bar{E} \sigma_m(\bar{E}, z_m),
\]

(A7)

and shows that Eq. A2 can also be rewritten for effective values.

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Note: The type of trap states considered by AM might correspond to Si–Si weak bonds, which act like donors, i.e. being either neutral or positively charged. If the energetic position is deep inside the energy gap, it can also be seen as a hole trap state.

Note: In this work we calculate the Fermi energy inside the 2D layer according to the electron density $n_s$. AM have considered two different cases in their work, the one discussed before is their case (B), whereas their case (A) assumes that the Fermi energy (chemical potential) of the 2DES and the Si substrate coincide and show the same temperature dependence. We do not consider case (A) in detail, as we think that case (B) is more realistic.

Note: The weighting of $\tau(E)$ with the kinetic electron energy $E$ in Eq. A1 fundamentally follows from the Drude-Boltzmann approximation as the Fermi velocity $v_F$ and the shift of the Fermi surface in k-space are both proportional to $\sqrt{E}$, which enter into the expression for the current $j_x = -e \int d\vec{k} n(\vec{k}) f(E)v_x$. The integral in the denominator of Eq. A1 in 2D is just equal to the Fermi energy $E_F$ — also for elevated temperatures.

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