Interface steps in field effect devices

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The charge doped into a semiconductor in a field effect transistor (FET) is generally confined to the interface of the semiconductor. A planar step at the interface causes a potential drop due to the strong electric field of the FET, which in turn is screened by the doped carriers. We analyze the dipolar electronic structure of a single step in the Thomas-Fermi approximation and find that the transmission coefficient through the step is exponentially suppressed by the electric field and the induced carrier density as well as by the step height. In addition, the field enhancement at the step edge can facilitate the electric breakthrough of the insulating layer. We suggest that these two effects may lead to severe problems when engineering FET devices with very high doping. On the other hand steps can give rise to interesting physics in superconducting FETs by forming weak links and potentially creating atomic size Josephson junctions.

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I. INTRODUCTION

The field effect transistor is a widely used device, both for commercial products as well as in research on correlated electron system (a recent overview is given in Ref. [1]). Traditionally this technique is applied to semiconductors, such as silicon or GaAs, and more recently to high temperature superconductors (see Ref. [2] and references therein) as well as organic materials [3,4,5,6,7,8]. The field effect is intriguing because it allows in principle to tune the charge density continuously by changing the applied voltage between gate and source/drain (see Fig. 1). However, field effect experiments on the systems mentioned above are difficult, because high electric fields, limited by the electric breakdown of the insulating dielectric, are required in order to achieve substantial changes of the charge distribution. Nevertheless, new gate insulator materials, such as complex oxide dielectrics and ferroelectric oxides, in recent years allowed to push induced surface charge densities to promising values. Thereby operating a FET at high electric fields leads to a strong confinement of the induced surface charge to the dielectric-semiconductor interface. Therefore, imperfections of the interface become important.

In the present paper the effect of interface steps in such devices is considered. Steps occur as imperfections when growing crystals, or can be created artificially. Naturally, one expects that steps act as barriers in the transport channel confined to the surface. Below we show under what circumstances this effect should be important, and that the transmission through the step depends exponentially on the electric field and the step height. Therefore, at high enough doping, a step cuts the transport channel and may present a severe problem. This may be particularly important in organic FETs where the step height is given by the molecular size and therefore is quite big. However, in superconducting FETs the step-barrier can act as a weak link and give rise to a Josephson junction where the critical current depends exponentially on the applied field. This might be an interesting way to design a dissipationfree switch in a superconductor [9].

We distinguish two types of field effect transistors. The term metal-insulator-semiconductor FET (MISFET) is used for a whole class of devices where the intrinsic carrier density of the semiconductor is negligible ($N_i \approx 0$) in the absence of the electric field. The electric field serves to induce a conducting space-charge layer on the surface (see Fig. 1). In contrast to this, in the superconducting FET (SUFET), the semiconductor is replaced by a superconductor or metal (above $T_c$) which has a finite density $N_i$. In this case the electric field alters the density which, for example, may change the superconducting $T_c$. In both cases the electric field induces a surface charge which screens the field. However, the extension $z_0$ of the surface charge perpendicular to the interface differs for MISFET and SUFET due to the difference in $N_i$. As a surface step of height $h$ is expected to be important for $h \gtrsim z_0$, we first give a rough estimate of $z_0$ for both cases.

The problem of the charge profile in MISFETs was extensively studied in Ref. [11] for the case of a continuous medium. Calculations for molecular crystals, which explicitly take into account the discreteness of the lattice, were done recently [12,13]. Below we follow Ref. [11] and refer to this work for more details. In the case of a perfectly flat and infinite interface, the wavefunction of the carriers can be separated into a plane-wave part parallel to the interface and a transverse part $\zeta(z)$, where the $z$-direction is perpendicular to the interface. The charge profile is then given by $n(z) \propto \zeta(z)^2$. The transverse function $\zeta$ is best calculated using a trial wavefunction for the lowest subband, such as the Fang-Howard trial wavefunction $\zeta(z) \propto z \exp(-bz/2)$, where $b$ is the variational parameter. We use this ansatz which is sufficient for our purpose, although more accurate trial functions exist [14]. Minimizing the energy with respect to $b$ yields the average distance $z_0$ of the charge distribution from
In the equation above $\varepsilon$ is the dielectric constant of the semiconductor, $m_z$ its effective mass in the $z$-direction and $n_0$ the induced surface carrier density. Note that we use a small $n$ for surface density and a capital $N$ for the volume density. Estimates of $z_0$ are given in Tab. I Parameters for the Si-FET are standard and given in the literature. At the highest possible fields, $z_0 = 12 \, \text{Å}$, which corresponds to a few unit cells. Pentacene was chosen as an example for an organic MISFET, and the parameters for the thin film transistor presented in Ref. 2 were taken. Only the effective mass $m_z$ is not accessible by experiment and has to be estimated from band-structure calculations. Theoretical calculations yield a hopping $t_z = 0.47 \, \text{meV}$ between the Pentacene molecules in the $z$-direction. Assuming a tight-binding band, the effective mass at the minima of the band is given by $m_z = h^2/(2a^2 t_z)$, where $a = 15.5 \, \text{Å}$ is the layer spacing in the $z$-direction. This yields $m_z = 0.34 \, m_0$. Equation (1) gives then $z_0 = 20 \, \text{Å}$ which is of the same order as the layer spacing. Hence, molecular steps, as are observed when growing films, may be important in such devices. Note that up to now, pentacene samples used in the experiments have many traps which may lead to corrections to the estimation of $z_0$ in Eq. (1). However, there are experimental attempts to use single crystals in order to reduce the number of traps.

In the case of SUFETs the superconductor has a finite density $N_s$ of carriers which give raise to metallic screening. Electric fields are screened within the Thomas-Fermi screening length $\lambda_T$. Therefore $z_0 \approx \lambda_T$ for SUFETs. In cuprates (e.g. $\text{YBa}_2\text{Cu}_3\text{O}_7$) $N_s \approx 1.5 \times 10^{21} \, \text{cm}^{-3}$ and the Thomas-Fermi screening length is estimated to be $5-10 \, \text{Å}$ (Ref. 2). This is larger than the width of the superconducting layer (3 Å), but smaller then the unit cell ($a = 15 \, \text{Å}$), which means that only the first superconducting layer is affected by the electric field. Therefore, it is important that the transport in the SUFET occurs only in the first layer. Note that in a SUFET the drain and source electrodes usually contact the first layer (see Fig. 1). However, the Josephson coupling among layers is increased in order to suppress the Josephson coupling. (c) The interlayer Josephson coupling is suppressed e.g. by a parallel magnetic field (Fraunhofer like pattern). In Ref. 11 possibility (a) was realized and changes in $T_c$ as well as an insulating phase were induced by the field effect. The ferroelectric Pb(Zr$_x$Ti$_{1-x}$)O$_3$ was used as a gate dielectric and a surface carrier density $n_0 = 7 \times 10^{13} \, \text{cm}^{-2}$ was achieved. The superconductor consisted of 1 to 2 unit cells of $\text{GdBa}_2\text{Cu}_3\text{O}_{7-\delta}$. Similarly, a single superconducting $\text{CuO}_2$-layer has been created due to inhomogeneous oxygen doping (resulting in a distribution of $T_c$ in the layers) on the surface of a $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ single crystal in Ref. 18. Again, in this device the physics is confined to a small region at the interface and steps should play an important role. In particular, when the sample is superconducting, a step may induce a weak link. This effect can be of particular relevance in highly anisotropic layered superconductors such as the high-$T_c$ material $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ or intercalated (LaSe)$_{1.14}$NbSe$_2$, see Ref. 19 where the thickness/coherence length $\xi \approx 3 \, \text{Å}$ of the superconducting ($\text{CuO}_2$ or NbSe$_2$)-layers is much smaller than their distance ($d \approx 15 \, \text{Å}$), i.e. atomic-size steps can naturally constitute a weak link (case b).

In the following we solve first the problem of an interface step of a perfect conductor exposed to a perpendicular electric field. This is a good approximation for $h \gg z_0$ and yields an induced dipole. Knowing the charge dipole, the potential barrier across the step is calculated using the Thomas-Fermi approximation. Finally, the transmission coefficient for tunneling through the step is calculated in the WKB approximation.

**II. PERFECT CONDUCTOR APPROXIMATION**

In the geometry with a step of height $h$ along the $y$-direction (see Fig. 2) we model the interface by a two-dimensional grounded conductor with a potential difference $V_G$ to the gate in distance $d$. This approximation becomes exact, if the thickness of the charged area is small compared to the step height, $z_0 \ll h$. Far from the step the electric field is homogenous, $E_0 = V_G/d \approx V_G/(d+h)$, but it is distorted near the step, as a surface charge is induced there in order to compensate the potential difference $\Phi_0 = eV_Gh/d$, which is realized for a flat interface with a homogeneous charge distribution. The typical equipotential curves near the step are shown in Fig. 3.

As the system is invariant in the $y$-direction, we can use the conformal transformation (in the $xz$-plane)

$$u = x + iz = \frac{h}{\pi} \left[ \sqrt{w^2 - 1} + \log \left( w + \sqrt{w^2 - 1} \right) \right],$$

where $w = \sqrt{z^2 - z_0^2}$.
TABLE I: Comparison between different FETs. $\varepsilon_d$ and $\varepsilon_s$ are the dielectric constants of the dielectric and the semiconductor, respectively. $m_s$ is the effective mass in the $z$-direction which enters equation (1). $N_i$ is the intrinsic carrier density. $E_b$ is the sample dependent breakdown field and $n_0 = E_b \varepsilon_d / (4 \pi \varepsilon)$ is the maximum surface carrier density. $z_0$ is the distance from the charge distribution from the interface, which is calculated by Eq. (4) for the MISFET and equal to the Thomas-Fermi screening length $\lambda_{TF}$ in the case of the SUFET. $h$ is the step height which, for Pentacene and GdBa$_2$Cu$_3$O$_{7-x}$, was taken to be the layer spacing in the $z$-direction. $n_i = N_i h$ is the intrinsic surface carrier density in a single layer. $k_F = \sqrt{2 \pi (n_i + n_0)}$ is the Fermi-wave vector. $(T)$ is the average transmission coefficient calculated by equation (4). $b^a$ See text, $b^b$ Ref. 1. $b^c$ Ref. 2. $b^d$ Ref. 3. $b^e$ Ref. 4.$b^f$ Ref. 5.$b^g$ Ref. 6.

$| \Phi(x, z) | = \frac{E_0 h}{\pi} \text{Im}[w(u = x + i z)]. \quad (4)$

Far from the step, $w(u)$ from equation (4) can be expanded in orders of $h/\sqrt{x^2 + z^2}$, which yields the approximate expression

$\Phi(x, z) = -E_0 \left( z - h \frac{x}{\theta(x, z)} \frac{1}{\pi} \right), \quad \sqrt{x^2 + z^2} \gg h, \quad (5)$

where $\theta$ is the polar angle in the $xz$-plane. In general, the surface charge of a perfect conductor is given by

$\Phi(x, z) = -E_0 \left( z - h \frac{\pi}{\theta(x, z)} \right), \quad \sqrt{x^2 + z^2} \gg h, \quad (5)$

which maps the upper half complex plane onto the domain above the step, the cuts being on the positive real axis. The solution for the potential is then given by

$n = \varepsilon_d E_\perp / (4 \pi \varepsilon), \quad E_\perp$ is the electric field being perpendicular to the interface and $\varepsilon_d$ is the dielectric constant of the gate insulator. Using equation (6) for the potential yields the asymptotic charge distribution $(x \gg h)$

$n(x) = n_0 \left( 1 - \frac{1}{\pi} \frac{1}{x} \right), \quad (6)$

with the doping $n_0 = \varepsilon_d E_0 / (4 \pi \varepsilon)$. The exact solution is given by the parametric expression

$n(x, z) = n_0 \left[ 1 - \frac{w(u)}{1 + w(u)} \right]^{1/2}, \quad (7)$

where $w(u)$ is given by Eq. (4) and $u = x + i z$ is taken on the surface of the conductor. The exact result as well as the approximation equation (6) are shown in Fig. 4. Obviously, the electric field induces a dipole center at the step which falls off as $x^{-1}$ far from the step.

It can be shown by the exact solution (7) that there is a weak divergence ($\sim x^{-1/3}$ or $\sim (h - z)^{-1/3}$ respectively) of the surface charge at the upper corner of the step due to the sharp edge, which enhances the local tunneling rate through the dielectric and can therefore serve as a nucleation center for a possible breakthrough of the device. The singularity at the edge can be regularized: (a) at distances from the step smaller than the local $\lambda_{TF}$, where the quantum mechanical exclusion principle comes into play, (b) geometrically due to finite step curvature. In both cases the field enhancement is of the order $(h/\lambda_c)^{1/3}$ where $\lambda_c$ is the cutoff ($\lambda_{TF}$ or finite curvature) which is at least of the order of the atomic scale ($\lambda_c \approx 1 - 2 \AA$). Hence, ratios $h/\lambda_c$ might be of the order 10 − 20 and the field enhancement is expected to be a factor $2 - 3$. This is not a big factor, but it should nevertheless be important, because steps are line defects which have a big probability to hit a “weak spot” in the dielectric where an electric breakthrough can occur. Note also...
that kinks in the step would lead to a further enhancement of the electric field. (c) The singularity can also be regularized due to the finite bandwidth, where the locally induced charge exceeds the filling of the band. This occurs when the potential difference \( \Phi_0 = eV_c h/d \) exceeds the bandwidth. For the maximal gate fields \( \Phi_0 = E_g h \) which is 2 eV for the Si-MISFET and 0.5 eV for the pentacene MISFET (see Tab. I). In the latter case this is roughly the bandwidth and a complete local charge depletion can be expected\(^{15}\).

III. TRANSMISSION ACROSS THE STEP

As discussed in the introduction, the wavefunctions of the electrons confined to a flat and infinite interface can be separated into a parallel and a transverse part: \( \psi_{kj}(r,z) = e^{i(k_r r + k_z z)} \) where \( r = (x,z) \) and \( k = (k_x, k_z) \) represent coordinate and wavevector parallel to the interface and \( j = 0, 1, 2 \ldots \) labels the discrete and confined states in the transverse direction. The energies are given by

\[
\epsilon_{kj} = \frac{\hbar^2 k^2}{2m_\parallel} + \epsilon_j. \tag{8}
\]

It can be shown that the eigenvalues \( \epsilon_j \) of the transverse part scale as \( \epsilon_j \propto E_0^{2/3} \propto n_0^{2/3} \), where \( E_0 \) and \( n_0 = \epsilon_g E_0/(4\pi e) \) are the electric field and the surface carrier density respectively (see Ref. 11). If only the \( j = 0 \) state is occupied (i.e. the lowest subband), then the system is two-dimensional and the Fermi energy is given by \( \epsilon_F = n_0 g \), where \( g = m_\parallel/(\pi \hbar^2) \) is the constant density of states. The condition for the occupation of only the lowest subband is \( \epsilon_F < \epsilon_1 - \epsilon_0 \) which holds for densities \( n_0 \) below a certain threshold. In Si, this threshold is \( 3 \times 10^{13} \text{ cm}^{-2} \) (using the triangular potential approximation, see Ref. 11) which is of the same order as the maximally achievable surface densities (see Tab. I). Hence, it is not clear, whether only the lowest subband is occupied. However, the presence of a step leads to charge dipole which suppresses the carrier density on the lower side of the step where the condition is then clearly satisfied. As discussed below, it is exactly this region which is of interest when calculating the transmission coefficient through the step. Therefore, we consider in the following only the lowest subband and treat the system as two-dimensional. The non-uniform charge distribution, caused by the step, can be treated in the Thomas-Fermi approximation (TFA) which locally assumes a free (here 2D) electron gas with density

\[
 n(r) = g \epsilon_F (r) = g [\epsilon_F - V_{\text{loc}}(r)], \tag{9}
\]

where \( \epsilon_F(r) \) is the spatially dependent Fermi Energy. At this point the result of the previous section enters by assuming that the surface carrier density \( n(r) = \int dz N(r,z) \) of the real system is still well approximated by the perfect conductor approximation (PCA). Note that in the PCA the induced charge is a pure surface charge with zero width and therefore differs from the real charge distribution which has a finite extension in the \( z \)-direction. However, the PCA becomes exact far from the step. Furthermore, knowing the solution of the PCA allows to calculate the local potential \( V_{\text{loc}} \) via relation (9). In the following the approximate solution (9) of the PCA is used which has the right asymptotics and which permits an analytic calculation of the transmission coefficient. Combining relations (9) and (9) yields

\[
 V_{\text{loc}}(x) = \frac{1}{\pi} \frac{n_0 h}{g} x = \frac{h^2 n_0}{m_\parallel} x. \tag{10}
\]

The potential (10) acts as a potential barrier across the step for \( x > 0 \). In the WKB approximation the transmission coefficient \( T(k) \) of a mode \( k \) is given by

\[
 T(k) = \exp \left( -2 \int_0^{x_0} \sqrt{(2m_\parallel/\hbar^2) [V_{\text{loc}}(x) - \epsilon_k]} \, dx \right), \tag{11}
\]

where \( \epsilon_k = \epsilon_{k_0} - \epsilon_0 - \hbar^2 k_x^2/(2m_\parallel) \) is the kinetic energy along the \( x \)-direction. Using the local potential (10) implies \( x_0 = n_0 h/\pi ge \) which yields the analytic result

\[
 T(k) = \exp \left( -2\pi n_0 \frac{h}{|k_x|} \right). \tag{12}
\]

Not surprisingly, the transmission coefficient depends exponentially on the step height \( h \) and on the electric field which is proportional to the surface density \( n_0 \). In order to calculate the conductance through the step, the average \( \langle T \rangle \) over the Fermi surface of the transmission coefficient enters, which for the parabolic band is

\[
 \langle T \rangle = \int_0^{2\pi} \frac{d\varphi}{2\pi} T(k_F \cos \varphi) = f \frac{2\pi n_0 h}{k_F}, \tag{13}
\]
where the function $f$ is given by

$$f(x) = \frac{2}{\pi} \int_{0}^{\pi/2} d\varphi e^{-x/\cos\varphi} \approx \frac{2}{\pi} \frac{e^{-x}}{\sqrt{x}}.$$  \hspace{1cm} (14)

The approximate expression is valid for $x \gg 1$. In a 2D system with parabolic dispersion the Fermi wave-vector is $k_F = \sqrt{2\pi(n_i + n_0)}$, where $n_i$ is the intrinsic carrier density. In the MISFET $n_i = 0$ which yields the simple expression $(T) = f(k_F h)$. The conductance through the step is given by the Landauer Formula

$$G = G_0 \frac{N}{T},$$  \hspace{1cm} (15)

where $G_0 = 2e^2/h \approx 12.9$ kΩ is the quantum conductance. $N = (2/\pi) k_F L$ is the number of channels for a sample of size $L$ (along the $y$-direction) taking into account both spins and the condition $-k_F < k_y < k_F$. The functional behavior of $f$ implies that the conductance through steps with height $h > k_F/(2\pi n_0)$ (in the MISFET $h > 1/k_F$) are exponentially suppressed.

Equation (15) was applied to the FET examples discussed previously and the results are summarized in Table I. An arbitrary step height $h = 20 \text{ Å}$, which might be due to an artificial step, was taken for the Si-MISFET, which yields $(T) = 0.06$ for the highest fields. In the Pentacene MISFET where $1/k_F = 15 \text{ Å}$ which is almost the same as the interlayer spacing ($a = 15.5 \text{ Å}$) and which yields $(T) = 0.2$ for a molecular step ($h = a$) at the highest achievable dopings.

Recently, there were unconfirmed claims that pentacene would become superconducting when doped to half filling.\textsuperscript{20} In the light of our discussion such high dopings are unlikely, as the locally enhanced electric field at the step edges might lead to the electric breakdown in the dielectric. Even if such electric fields could be reached in reality, the resulting device would be significantly limited by molecular steps, as for required density $n_0 = 2 \times 10^{14} \text{ cm}^{-2}$ corresponding to $1/k_F = 3 \text{ Å}$ the transmission $(T) = 2 \times 10^{-5}$ of the step would be small.

In lower electric fields, for the SFET below $T_c$, the charge dipole due to the step can form a Josephson junction, which is of the SIS or SNS-type depending on the charge density in the nonsuperconducting region. The critical current $I_c$, through this junction can be estimated for a SNS tunnel junction by the Ambegaokar-Baratoff formula\textsuperscript{21}

$$I_c R = I_c G^{-1} = \frac{\pi \Delta}{2e} \tanh \left( \frac{\Delta}{2kT} \right),$$  \hspace{1cm} (16)

where $\Delta$ is the (s-wave) gap of the superconductor and $G$ the conductivity from equation (15). In this case the critical current $I_c$ depends on the external electric field exponentially via the effective thickness of the insulating region, which enters the tunnel matrix element $T$. A similar exponential dependence $I_c \sim \exp(-l/l_T)$ is found in field effect doped SNS-junctions with a large distance $l$ of the superconducting leads, $l \gg l_T = (\hbar D/2\pi k_B T)^{1/2}$ \textsuperscript{(16)} (D $\sim n^{1/2}$ Diffusion constant in normal metal), while in the opposite limit $l \ll l_T$ the critical current depends algebraically on $l$, $I_c \sim l$, see Ref. \textsuperscript{22}. In both cases it is seen that the superconducting transport depends sensitively on the local charge density near the step, i.e. can be easily modified by an external electric field.

Note that in a highly anisotropic layered superconductors, such as high-$T_c$-materials an atomic size step can already form a weak link in the absence of the charge dipole effect described here, because the coherence length ($\xi = 3 \text{ Å}$) of the quasi 2D superconducting layers is smaller than the height $h$ of the step.

To conclude, we showed that a charge dipole is induced in the 2D electron gas near an interface step, which can lead to a Josephson weak link due to the local depletion of the charge density. This forms the limiting factor for transport through an ultrathin metallic or superconducting layer and might be used for ultrasmall dissipationfree switches (SUFET). In addition to this, the field enhancement near the step in the insulating barrier can trigger the breakthrough of the dielectric and thereby limit the maximal doping level $n_{0,\text{max}}$. Both effects are hard to avoid and pose a fundamental challenge in term of atomically flat interfaces for any FET device with a quasi 2D (super)conducting charge density.

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