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Voltage drop in the experiments of scanning tunneling microscopy for Si

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It is shown that the applied voltage to keep a tunnel current between a metallic tip and a semiconductor surface drops mainly in the semiconductor bulk and that diffusion plays an important role in the conduction process. Calculations for the case of Si(111)7×7 agree with experimental results for samples of very different doping.

In a recent paper, Binnig, Rohrer, Gerber, and Weibel have reported the observation of the (7×7) reconstruction on Si(111) by scanning-tunneling microscopy[1] (hereafter I). The experiment was performed by applying a tip-positive tunnel voltage of 2.9 eV, since voltages lower than 2.5 eV led to direct contact between tip and sample. This is in contrast to metals configurations, for which tunneling is observed for voltages as low as 0.01 eV.[2]

The purpose of this Rapid Communication is to show that in I practically all the applied voltage drops in the semiconductor and is closely related to the number of carriers.

Let us consider the experimental conditions for the semiconductor sample. Using an *n*-type crystal having a resistivity $\rho = 100\ \Omega$ cm (300 K), the experiment was performed under the following conditions:[3] V (tip-positive tunnel voltage) $= 2.9$ eV; intensity $= 5$ nA; $T \sim 300\,°\mathrm{C}$.

Those data correspond to a number of donors N_D less than $10^{14}\ \mathrm{cm}^{-3}$. For $T \sim 300\,°\mathrm{C}$, the *bulk* material becomes *intrinsic* with $n_i \simeq p_i \simeq 2\times 10^{15}\ \mathrm{cm}^{-3}$ ($\rho \simeq 10\ \Omega$ cm), although it has an *n*-type conductivity due to the three times greater electron mobility.

Consider the carrier conduction near the contact tunneling point. As is well known, the field lines near this contact point open out producing a spreading resistance that can be written approximately as

$$R \sim \rho \frac{l}{s} \ , \tag{1}$$

ρ being the semiconductor resistivity, and l and s the effective length and section of the current lines spreading near the contact, respectively. Estimations[4] of these values lead to $l \simeq 10$ Å, and $s \simeq 25\ \text{Å}^2$ (this area is related to the resolution of the experimental data and is approximately twice the area per surface atom). Then, for $n_i \simeq p_i \simeq 2\times 10^{15}\ \mathrm{cm}^{-3}$, $R \sim 4\times 10^{8}\ \Omega$ which matches experiment I. Here, we should stress that at $T = 300$ K the n and p concentrations drop dramatically, the material becomes extrinsic, and the resistivity ρ increases by a factor of 10. This corresponds to a voltage drop of 25 eV; for much lower voltages, other effects may appear, for example, tunneling from the valence band to the surface states can be important as well as field-emission effects (see Fig. 1). Therefore, high temperatures are quite necessary to perform the experiment, i.e., for high temperatures the voltage drop in the semiconductor is smaller.

For the high fields applied near the contact, the carriers do not have the time to lose the energy they gain from the electric field, producing a charge region near the point of contact, extending around 300 Å (see Fig. 1), the carrier mean-free path λ. This charge or spreading region can be analyzed by assuming spherical symmetry around the point of contact; to this end we use Poisson's equation:

$$\nabla^2 \phi = -4\pi\rho(\vec{r}) \ , \tag{2}$$

where the carrier charge $\rho(r)$ is related to $\vec{r}$, the distance to the point of contact, by the continuity equation

$$2\pi r^2 \rho(r) v(r) = I \ . \tag{3}$$

Here, $v(r)$ is the carrier velocity determined by the electric potential $\phi(r)$ and I the tunnel intensity. For a tip-positive voltage, the charge region attracts electrons due to the voltage drop near the contact (Fig. 1), and the hole channel is closed to the tunneling process, the reason being that at the contact holes can only be excited thermally, this effect creating a negligible current due to the *small contact area*. Then, $\rho(r)$ in Eqs. (2) and (3) corresponds to those electrons moving across the charge region. A good approximation to the solution of Eqs. (2) and (3) can be obtained by taking $v(r)$ as a constant, since the change of ρ with r is mostly due to the geometrical factor $2\pi r^2$. The solution to Eq. (2) has a term of the form $RI1/r$ (associated to the spreading resistance, and determined by the boundary conditions related, at $r \simeq \lambda$, to the bulk resistivity) and a correction due to the electron density in the space of charge

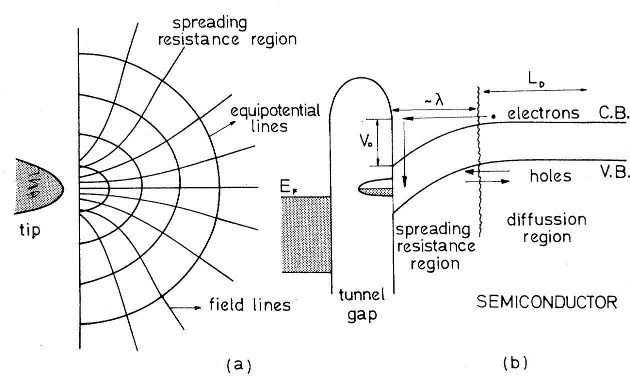

FIG. 1. Tip-semiconductor geometry. (a) Field lines open out from the point of contact. (b) For tip-positive voltage, electrons in the conduction band (C.B.) are attracted towards the point of contact, crossing the spreading resistance region and being trapped by the surface states. The diffusion region, characterized by the length L_D is much larger than the spreading resistance region.

or spreading resistance region. This effect tends to decrease only slightly (0.1 eV) the voltage drop due to the term $RI1/r$, and so Eq. (1) is a good approximation to the spreading resistance.

Note that for tip-negative voltages, the electron channel is now closed and the current near the surface is only due to holes. This can only happen if a diffusion process, extending through a diffusion distance L_D,[5] appears for $r > \lambda$. The diffusion equations for an intrinsic semiconductor are the following:[5]

$$-\frac{\Delta p_i}{\tau} + D\nabla^2(\Delta p_i) = 0 \ , \tag{4}$$

$$\Delta p_i = \Delta n_i \ , \tag{5}$$

where τ is the recombination lifetime for carriers and $D = D_h D_n/(D_h + D_n)$ (D_h and D_n are the diffusion coefficients for holes and electrons, respectively); Δp_i and Δn_i are the changes introduced in the intrinsic concentrations n_i and p_i by the diffusion process. From Eqs. (4) and (5), and by assuming spherical symmetry, we obtain the following results:

$$\Delta n_i = \Delta p_i = \nu \frac{e^{-r/L_D}}{r/L_D} \ , \tag{6}$$

where[5] $L_D = (D\tau)^{1/2} \sim 10^{-2}$ cm; ν is a constant to be determined by the boundary conditions at $r \simeq \lambda$, for $\vec{j}_e$ and $\vec{j}_h$, the density currents for electrons and holes, respectively:

$$\vec{j}_e(r) = eD_n \vec{\nabla} n(r) + e\mu_e \vec{E}(r) \ , \tag{7a}$$

$$\vec{j}_h(r) = -eD_h \vec{\nabla} p(r) + e\mu_h \vec{E}(r) \ , \tag{7b}$$

where μ_e and μ_h are the electron and hole mobilities, respectively, and $n = n_i + \Delta n_i$, $p = p_i + \Delta p_i$.

For a tip-positive potential, we impose the following condition: $j_h(r \simeq \lambda) = 0$; this equation determines ν and, finally, by using Eq. (7a), we obtain the following equation for the total density current $j = j_e + j_h$:

$$j(r \simeq \lambda) = \frac{2b}{b+1} e(n_i\mu_e + p_i\mu_h)E(r \simeq \lambda) \ , \tag{8a}$$

where $b = \mu_e/\mu_h$.

For a tip-negative potential (with the electron channel closed), we apply a similar analysis $[j_e(r \simeq \lambda) = 0]$, and obtain the result:

$$j(r \simeq \lambda) = \frac{2}{(b+1)} e(n_i\mu_e + p_i\mu_h)E(r \simeq \lambda) \ . \tag{8b}$$

These equations show that, for a given intensity, the electric field at $r \simeq \lambda$ for the tip-negative voltage is b times greater than the one obtained for a tip-positive voltage. This result shows that, for a negative voltage, the spreading resistance must be b times larger. This can be an experimental check to our discussion. [Note that Eqs. (8a) and (8b) determine $E(r)$ at $r \simeq \lambda$, and give the voltage drop across the space of charge or spreading resistance region (see above).]

What will happen to an extrinsic case? The argument runs as before, but now the extrinsic bulk resistivity has to be calculated with the given number of donors or acceptors. A little change appears with respect to the intrinsic case when the current density is related to the applied electric field. Now, the equations for the changes Δn_0 and Δp_0 introduced in the extrinsic concentrations n_0 and p_0 are[5]

$$-\frac{\Delta n_0}{\tau} + D_n\nabla^2(\Delta n_0) + \mu_e \vec{E} \cdot \vec{\nabla}(\Delta n_0) = 0 \ , \tag{9a}$$

$$\Delta n_0 = \Delta p_0 \ , \tag{9b}$$

if we assume $n_0 << p_0$ (a similar equation for the case $n_0 >> p_0$ can be also written). The conditions under which the experiments are performed imply that the effect of the electric field is small compared with the diffusion process. Under these conditions, Eqs. (9a) and (9b) reduce to two equations similar to Eqs. (4) and (5) in such a way that the analysis given above for the intrinsic semiconductor can be also applied to the extrinsic case. From this analysis, we have obtained the following results.

(i) Tip-positive voltage (hole channel closed):

$$(a)\ p_0 >> n_0,\ j(r \simeq \lambda) = bqp_0\mu_p E(r \simeq \lambda) \ , \tag{10a}$$

$$(b)\ n_0 >> p_0,\ j(r \simeq \lambda) = qn_0\mu_e E(r \simeq \lambda) \ . \tag{10b}$$

(ii) Tip-negative voltage (electron channel closed):

$$(a)\ p_0 >> n_0,\ j(r \simeq \lambda) = qp_0\mu_p E(r \simeq \lambda) \ , \tag{11a}$$

$$(b)\ n_0 >> p_0,\ j(r \simeq \lambda) = \frac{1}{b} qn_0\mu_e E(r \simeq \lambda) \ . \tag{11b}$$

Note the different factors appearing in the relation between j and E, although in all the cases we find, for a tip-negative voltage, a three times greater electric field, assuming $b \sim 3$, and a corresponding increase in the spreading resistance. For example, the sample can be doped with high values of acceptors; then, according to (10a), we find that, for a given intensity and tip-positive voltage, the electric field $E(r \simeq \lambda)$ is proportional to one-third of the bulk resistivity, while in the intrinsic case we found a factor of $\frac{2}{3}$: this introduces a factor of $\frac{1}{2}$ for the spreading resistance of an extrinsic semiconductor, as compared with the intrinsic case.

It is worth commenting at this point that this analysis applies even for high extrinsic dopings. Indeed, the limitation to the previous discussion comes from the availability of the minority carriers to keep a certain diffusion current: for $\Delta n_0 \simeq 10^{12}$ cm^{-3}, at $r \simeq \lambda$, the total diffusion intensity $2\pi r^2 eD_n \vec{\nabla}(\Delta n)$ at $r \simeq \lambda$, as obtained from an equation similar to Eq. (6), is close to 10^{-7} A. This shows that Δn_0 at $r \simeq \lambda$ is around 10^{10} cm^{-3}, and that no limitation appears to our analysis for moderate or even high dopings.

Binnig, Rohrer, Salvan, and Baró[3] have performed recently an experiment with extrinsic p doping, having the following room-temperature resistivity $\rho = 1\ \Omega$ cm. Tunneling was observed for $T = 440$ K with an applied voltage of around 0.2 eV ($I = 5$ nA), which is much smaller than in the intrinsic case. These results fit our previous analysis since for $T = 440$ K, $\rho \simeq 2.6\ \Omega$ cm due to the decrease in the mobility (the number of carriers 10^{+16} cm^{-3} is practically unaffected by temperature). This resistivity is four times lower than the one found above for the intrinsic semiconductor at $T \simeq 300$ °C; by including the $\frac{1}{2}$ factor discussed after Eq. (10a), we conclude that the spreading resistance is approximately eight times lower for the actual extrinsic case. This leads to a drop voltage of 0.3 eV, in good agreement with experiments.

We conclude the following.

(1) The applied voltage in the tip-semiconductor tunnel

process drops mainly in the semiconductor and is reduced by increasing the carriers concentration.

(2) Tip-positive potentials present resistances around three times (the ratio between the electrons and holes mobilities) smaller than tip-negative voltages.

(3) Spreading resistances are reduced by decreasing the bulk resistivity by changing the temperature and/or carrier concentration.

(4) Diffusion processes play a very important role in maintaining the currents.

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