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# Influence of the Si/SiO<sub>2</sub> interface on the charge carrier density of Si nanowires

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**ABSTRACT** The electrical properties of Si nanowires covered by a SiO<sub>2</sub> shell are influenced by the properties of the Si/SiO<sub>2</sub> interface. This interface can be characterized by the fixed oxide charge density  $Q_f$  and the interface trap level density  $D_{it}$ . We derive expressions for the effective charge carrier density in silicon nanowires as a function of  $Q_f$ ,  $D_{it}$ , the nanowire radius, and the dopant density. It is found that a nanowire is fully depleted when its radius is smaller than a critical radius  $a_{crit}$ . An analytic expression for  $a_{crit}$  is derived.

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## 1 Introduction

The potential use of silicon nanowires as parts of future devices has triggered an increased interest in silicon nanowire research. The application of silicon nanowires, however, requires well defined electrical properties and this is a subtle problem as surface charges are known to influence the charge carrier density of semiconductors [1]. This is especially problematic for nanowires, which, due to their rod-like geometry and their nanoscale dimensions, have an extremely large surface-to-volume ratio. Consequently, their properties might be strongly influenced by the nanowire surface; an effect which is sometimes considered [2–7] but often neglected [8–10].

Silicon is known to oxidize rapidly in air, thus considering the electrical properties of silicon nanowires, the influence of charges located within the SiO<sub>2</sub> shell and/or at the Si/SiO<sub>2</sub> interface have to be taken into account. It is the scope of this paper to discuss the influence of the Si/SiO<sub>2</sub> interface on the charge carrier density of silicon nanowires. Expressions for the effective charge carrier density of a silicon nanowire as a function of the nanowire radius, the doping concentration and the interface charge density will be derived.

## 2 Silicon/silicon dioxide interface properties

Silicon nanowires are usually covered by an SiO<sub>2</sub> shell. According to the most commonly used nomenclature [11], one distinguishes between electric charges located

deep inside the SiO<sub>2</sub> shell and charges located at or in close vicinity of the Si/SiO<sub>2</sub> interface. Charges inside the SiO<sub>2</sub> layer are classified as oxide trapped charges or mobile ionic charges with respective densities  $Q_{ot}$  and  $Q_m$ .

Charges at or in close vicinity of the Si/SiO<sub>2</sub> interface, can also be subdivided into two categories: the fixed oxide charge density  $Q_f$ , and the interface trap charge density  $Q_{it}$ . In the following discussion we will concentrate on the effect of  $Q_f$  and  $Q_{it}$  on the charge density of the nanowire, due to their stronger influence on the electric properties [12]. The fixed oxide charges, by definition, do not interact via a charge transfer with the underlying silicon so that  $Q_f$  does not depend on the position of the Fermi-level. Electron-spin-resonance studies showed that the trapped oxide charges may be partly attributed to so-called  $E'$  resonance centers, which are trivalent silicons, bonded to three oxygens [13–16]. Unlike the fixed oxide charges, the interface trap charges do interact via a charge transfer with the Si body of the nanowire. The interface trap charge density  $Q_{it}$  arises by charging interface states of level density  $D_{it}$  [ $\text{cm}^{-2}\text{eV}^{-1}$ ]. The nature of these interface states is closely related to the so-called  $P_b$  resonance centers, first observed by Nishi et al. [17–19] in electron-spin-resonance studies. These  $P_b$  centers could be identified as trivalent silicon atoms [19] bonded to three underlying silicon atoms [20, 21]. Extensive electron-spin-resonance studies on silicon/oxide capacitors showed that the  $P_b$  centers are the main cause for the presence of interface states [16, 20, 22–26], so that the characteristics of the interface traps is determined by the properties of the  $P_b$  centers. It was found that the  $P_b$  centers are amphoteric [16]. In the lower half of the bandgap a  $P_b$  center is donor-like ( $P_b \rightarrow e^- + P_b^+$ ), which means that, supposing the Fermi-level is located in the lower half of the bandgap, then the  $P_b$  centers below the Fermi-level are neutral, whereas the  $P_b$  centers between the Fermi-level and the bandgap middle are positively charged. The  $P_b$  centers in the upper half of the bandgap behave acceptor-like ( $P_b + e^- \rightarrow P_b^-$ ). If the Fermi-level is located in the upper half of the bandgap, the  $P_b$  centers between the Fermi-level and the bandgap middle are negatively charged, while the ones above the Fermi-level are neutral.

In addition to spin-resonance measurements, the interface trap level density was also determined by capacitance [12], and photovoltage measurements [27, 28], deep-level transient spectroscopy [26], measurements of the subthresh-

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old slope [29], irradiation and annealing studies [30–32], and simulations [33]. The outcome is that the density of Si/SiO<sub>2</sub> interface trap states is U-shaped, being approximately constant within a certain range of about  $\pm 0.25$  eV around the midgap (see [34, 35]). The magnitude of the interface trap level density can vary between approximately  $D_{it} = 1 \times 10^{10} \text{ cm}^{-2} \text{ eV}^{-1}$  and  $D_{it} = 1 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$ , depending on the oxidation and annealing conditions.

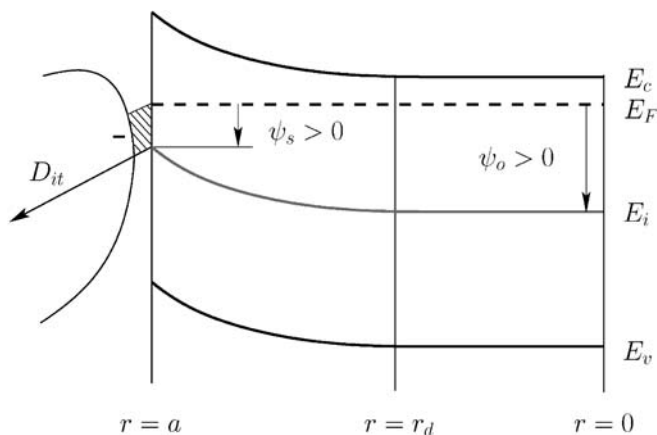
### 3 Theory

In the following, a model for the effective charge carrier density in a nanowire as a function of the interface trapped charge density  $Q_{it}$  and the fixed oxide charge density  $Q_f$  will be derived. To simplify the problem, we consider a circular slice of silicon of radius  $a$  covered by an oxide layer, which is equivalent to considering an infinitely long homogeneously doped cylindrical nanowire. Edge effects, like the diffusion of charge carriers from the substrate into the nanowire for example or the effect of metal contacts are neglected.

Figure 1 schematically depicts the radial band diagram of a circular slice of n-type silicon in the presence of interface traps of level density  $D_{it}$ , additionally assuming  $Q_f = 0$ . The Fermi-level  $E_F$  at the surface is located above the midgap level  $E_i$ , which corresponds to a positive surface potential  $\psi_s$ . As discussed before, the interface traps in the upper half of the bandgap between  $E_F$  and  $E_i$  will accept one electron each and become negatively charged (see the shaded region in Fig. 1). The necessary electrons are supplied by the n-type nanowire such that a depletion layer, extending from the nanowire surface at  $r = a$  to an inner radius  $r_d$ , develops. Within the depletion layer a net positive charge is present.

Defining the electrostatic potential  $\psi(r)$  in a way that it equals the midgap level  $E_i$ , taking the donors and acceptors of density  $N_D$  and  $N_A$  to be fully ionized, and employing the Boltzmann approximation, the charge density  $\rho(r)$  can be written as [34]

$$\rho(r) = q \left( p_0 \exp(-\beta\psi(r)) - n_0 \exp(\beta\psi(r)) + N_D - N_A \right), \quad (1)$$



**FIGURE 1** Schematic of the Si/SiO<sub>2</sub> interface and the radial band-bending of n-doped nanowire assuming  $Q_f = 0$ . The shaded area indicates filled interface trap levels of density  $D_{it}$  leading to a negative surface charge and a depletion of the nanowire in the region  $r_d < r < a$

with  $\beta = q/kT$ . The parameters  $n_0$  and  $p_0$  in the above equation are given by

$$n_0 = N_c \exp\left(-\frac{E_g}{2kT}\right), \quad (2)$$

$$p_0 = N_v \exp\left(-\frac{E_g}{2kT}\right), \quad (3)$$

where  $N_c$  and  $N_v$  are the density of states in the conduction and valence band, respectively. Furthermore, we will adopt the full depletion approximation, i.e. assuming an abrupt transition between the depletion layer and the non-depleted semiconductor material (neglecting charge carrier diffusion between the depleted and the non-depleted region) so that the charge density is approximated as

$$\rho = \begin{cases} 0 & 0 \leq r < r_d \\ q(N_D - N_A) & r_d \leq r \leq a \end{cases}. \quad (4)$$

By solving the Poisson equation in polar coordinates, the electrostatic potential  $\psi(r)$  can be obtained

$$\psi(r) = \begin{cases} \psi_0 & 0 \leq r < r_d \\ \psi_0 - \frac{q}{4\epsilon_s} (r^2 - r_d^2) & r_d \leq r \leq a \end{cases}. \quad (5)$$

According to the above equation, the potential at the silicon surface  $\psi_s = \psi(a)$  is

$$\psi_s = \psi_0 - \frac{q}{4\epsilon_s} (a^2 - r_d^2), \quad (6)$$

with  $\psi_0$  being the potential at  $r = 0$ . If the nanowire is only depleted at its surface, the charge density  $\rho$  vanishes for  $r \leq r_d$ . The value of the potential  $\psi_0$  can be obtained by setting (1) to zero and solving for  $\psi_0 = \psi(0)$  [12]

$$\psi_0 = \beta^{-1} \ln \left\{ \frac{N_D - N_A}{2n_0} \left( 1 + \left( 1 - \frac{2n_0 p_0}{(N_D - N_A)^2} \right)^{1/2} \right) \right\}. \quad (7)$$

Let us come back to the Si/SiO<sub>2</sub> interface and its properties. According to the definition, the interface charge density is given by the sum of  $Q_{it}$  and  $Q_f$ , where  $Q_f$  is constant and independent of the position of the Fermi-level. The interface trapped charges of density  $Q_{it}$  are assumed to have the same characteristic as the  $P_b$  centers, i.e. they are taken to be amphoteric. Furthermore, they are assumed to be neutral if  $E_F = E_i$ . Especially for high trap level densities  $D_{it}$  and low doping concentrations, the charge neutrality condition forces the Fermi-level at the nanowire surface to be located around midgap. Thus in this limit (high  $D_{it}$ , low doping) the situation could equally be described by pinning the Fermi-level at the nanowire surface at  $E_F = E_i$ . Approximating the Fermi distribution by a step function and assuming  $D_{it}$  to be constant around midgap,  $Q_{it}$  can be expressed as [28]

$$Q_{it} = -q^2 D_{it} \psi_s. \quad (8)$$

Charge neutrality provides another condition. Demanding that the nanowire slice is neutral, the space charge in the depletion layer has to equal the interface charge, which gives

$$\pi (a^2 - r_d^2) \rho + 2\pi a (Q_f + Q_{it}) = 0. \quad (9)$$

Using (6) and (8) and solving for the depletion radius  $r_d$  leads to

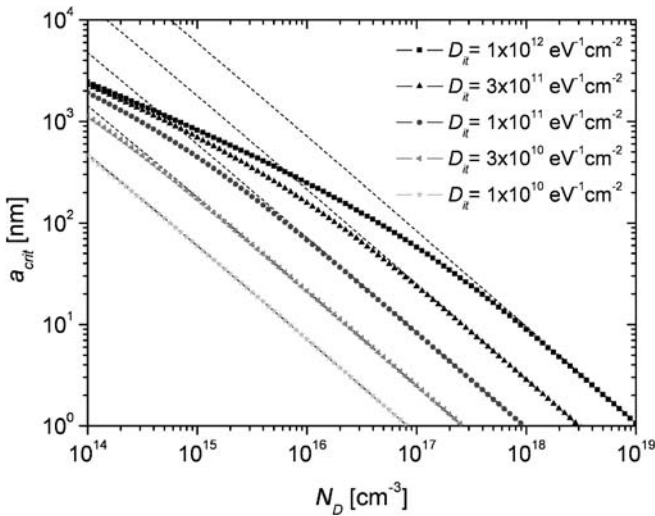
$$r_d = \sqrt{a^2 + \frac{2aQ_f - 2aq^2D_{it}\psi_0}{\varrho \left(1 + \frac{aq^2}{2\epsilon_s}D_{it}\right)}}. \quad (10)$$

One can see that for a specific set of parameters  $Q_f$ ,  $D_{it}$ ,  $a$ , and  $\psi_0$  the inner radius of the depletion layer can become zero. This defines a critical nanowire radius

$$a_{crit} = \frac{\epsilon_s}{q^2D_{it}} \left\{ -1 + \left[ 1 + \frac{4q^2D_{it}}{\varrho\epsilon_s} (q^2D_{it}\psi_0 - Q_f) \right]^{1/2} \right\}. \quad (11)$$

If the nanowire radius  $a$  is larger than  $a_{crit}$ , we face the situation that the nanowire is depleted at its surface, but still conductive in its center, see Fig. 1. If, however, the nanowire radius  $a$  is smaller than  $a_{crit}$  the nanowire is fully depleted. This is consistent with the observation of Calarco et al. for GaN nanowires [2]. Figure 2 shows the critical radius of an n-doped nanowire for different interface trap level densities  $D_{it}$  and zero fixed oxide charges ( $Q_f = 0$ ) as a function of the donor concentration  $N_D$ . The critical radius  $a_{crit}$  decreases with increasing doping concentration and decreasing  $D_{it}$ . This could be expected, since both, an increase of the doping, and a reduction of the interface trap level density reduces the width of the depletion layer. We can deduce from Fig. 2 that the doping of a silicon nanowire of 50 nm in diameter, assuming a medium trap level density of  $D_{it} = 1 \times 10^{11} \text{ eV}^{-1}\text{cm}^{-2}$  and zero  $Q_f$ , has to be larger than  $3 \times 10^{16} \text{ cm}^{-3}$  to prevent a full depletion of the nanowire. By expanding the square root of (11) to the first order we can obtain an approximated expression for  $a_{crit}$

$$a_{crit} \approx \frac{2}{\varrho} (q^2D_{it}\psi_0 - Q_f), \quad (12)$$



**FIGURE 2** Critical radius  $a_{crit}$  (according to (11)) as a function of the donor concentration  $N_D$  for different interface trap level densities  $D_{it}$ , assuming  $Q_f = 0$ ; *dashed lines* correspond to the approximated values for  $a_{crit}$  according to (12)

where  $\varrho = q(N_D - N_A)$  and  $\psi_0$  has to be determined by using (7). This formula seems sufficiently accurate for most practical cases. The obtained approximated values of  $a_{crit}$  are displayed in Fig. 1 as dotted lines.

Let us concentrate now on the influence of the interface charges on the charge carrier density. Depending on whether the radius is greater or smaller  $a_{crit}$ , we have to distinguish two cases. The first case corresponds to  $a > a_{crit}$ . Considering an n-doped nanowire, we can evaluate the effective electron concentration  $n_{eff>}$  (the greater sign indicates that  $a > a_{crit}$ ) by combining (2) and (5) and averaging over the nanowire area

$$\begin{aligned} n_{eff>} &= \frac{1}{a^2\pi} \int_0^a n_0 \exp(\beta\psi(r)) 2\pi r dr \\ &= \frac{2n_0}{a^2} \left\{ \int_0^{r_d} \exp(\beta\psi_0) r dr \right. \\ &\quad \left. + \int_{r_d}^a \exp\left(\beta\psi_0 - \beta\frac{\varrho}{4\epsilon_s}(r^2 - r_d^2)\right) r dr \right\} \\ &= n_0 \exp(\beta\psi_0) \left\{ \frac{r_d^2}{a^2} \right. \\ &\quad \left. + \frac{4\epsilon_s}{\beta\varrho a^2} \left[ 1 - \exp\left(\beta\frac{\varrho}{4\epsilon_s}(r_d^2 - a^2)\right) \right] \right\}, \quad (13) \end{aligned}$$

with  $\psi_0$  given by (7).

The second case corresponds to a fully depleted wire ( $a < a_{crit}$ ). The electrostatic potential can then be expressed as

$$\psi(r) = \psi_s + \frac{\varrho}{4\epsilon_s}(a^2 - r^2), \quad (14)$$

where the surface potential is determined by the charge neutrality condition

$$\psi_s = \frac{a\varrho + 2Q_f}{2q^2D_{it}}. \quad (15)$$

The effective electron density  $n_{eff<}$  for the fully depleted case ( $a < a_{crit}$ ) can be obtained by averaging the electron density over the nanowire area

$$\begin{aligned} n_{eff<} &= \frac{1}{a^2\pi} \int_0^a n_0 \exp(\beta\psi(r)) 2\pi r dr \\ &= n_0 \exp(\beta\psi_s) \frac{4\epsilon_s}{\beta\varrho a^2} \left[ \exp\left(\beta\frac{\varrho a^2}{4\epsilon_s}\right) - 1 \right]. \quad (16) \end{aligned}$$

Combining (13) and (16), we can evaluate the effective electron density  $n_{eff}$  for an arbitrary combination of  $N_D$ ,  $Q_f$  and  $D_{it}$ . Figure 3 shows  $n_{eff}$  for different interface trap level densities  $D_{it}$ , zero  $Q_f$ , and a radius  $a$  of 25 nm as a function of the donor density  $N_D$ . The characteristic feature of the curves is a sharp transition between a region of high and a region of low effective electron density. This transition is located at the  $N_D$  value, where the wire starts to be fully depleted. Similarly to Fig. 2, the onset of full depletion is shifted on the  $N_D$  axis depending on the density of interface trap levels. The smaller the

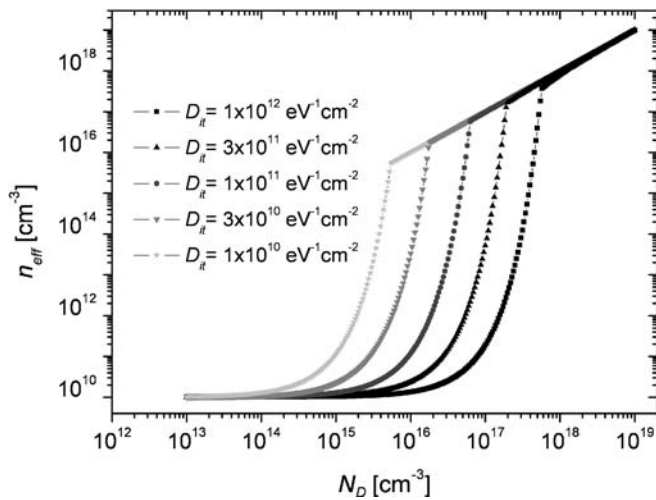


FIGURE 3 Effective electron densities  $n_{\text{eff}}$  for different values of  $D_{\text{it}}$ , assuming  $Q_f = 0$  and  $a = 25$  nm

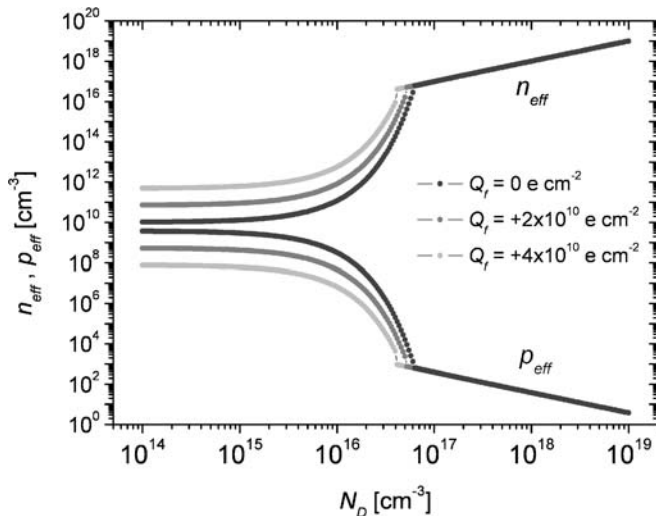


FIGURE 4 Effective electron and hole density,  $n_{\text{eff}}$  and  $p_{\text{eff}}$ , as a function of  $N_D$  for  $a = 25$  nm,  $D_{\text{it}} = 1 \times 10^{11} \text{ eV}^{-1} \text{ cm}^{-2}$  and different values of  $Q_f \geq 0$

$D_{\text{it}}$  value is, the smaller the doping concentration can be, without causing a full depletion of the nanowire. Since the fixed oxide charge was set to zero, the effective electron concentration approaches the intrinsic value of  $1.5 \times 10^{10} \text{ cm}^{-3}$  in the limit of low doping concentrations.

In order to demonstrate the effect of positive fixed oxide charges, Fig. 4 shows  $n_{\text{eff}}$  and  $p_{\text{eff}}$  as a function of  $N_D$ , assuming a medium interface trap level density ( $D_{\text{it}} = 1 \times 10^{11} \text{ eV}^{-1} \text{ cm}^{-2}$ ) and a nanowire radius of 25 nm. In the low  $N_D$  region, where the nanowire is fully depleted, the effective electron density is basically determined by the position of the surface potential. Equation (15) implies that a positive  $Q_f$  increases the surface potential and, concomitantly, the electron concentration. This can be seen in Fig. 4: in the limit of low doping concentrations,  $n_{\text{eff}}$  is greater than the intrinsic electron concentration.

Considering negative fixed oxide charges, the effect is reversed. As depicted in Fig. 5, a negative fixed oxide charge density,  $Q_f$ , leads for small  $N_D$ -values to an effective electron concentration,  $n_{\text{eff}}$ , that is smaller and an effective hole

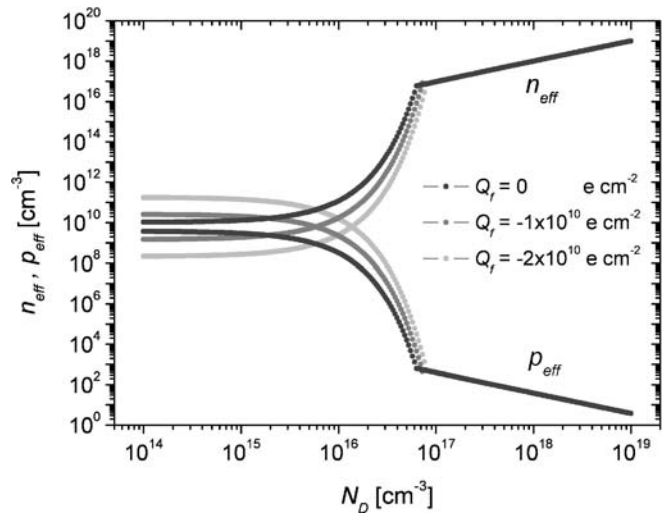


FIGURE 5  $n_{\text{eff}}$  and  $p_{\text{eff}}$  as a function of  $N_D$  for  $a = 25$  nm,  $D_{\text{it}} = 1 \times 10^{11} \text{ eV}^{-1} \text{ cm}^{-2}$  and different values of  $Q_f \leq 0$

density,  $p_{\text{eff}}$ , that is greater than the intrinsic one. Thus the nanowire is slightly inverted.

#### 4 Conclusion

To conclude, we have seen that, especially for nanowires of small radius, the interface trap level density  $D_{\text{it}}$  has a considerable influence on the effective charge carrier density. Depending on the interface trap level density, the doping concentration, and the nanowire radius  $a$ , the effective charge carrier density might be substantially lower than the doping concentration. We have derived an expression for a critical nanowire radius  $a_{\text{crit}}$ , which marks the border between nanowires that are fully depleted ( $a < a_{\text{crit}}$ ) and nanowires which are only depleted at their surface ( $a > a_{\text{crit}}$ ).

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