Tailoring the carrier mobility of semiconductor nanowires by remote dielectrics

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The dielectric environment of thin semiconductor nanowires can affect the charge transport properties inside the wire. In this work, it is shown that Coulomb impurity scattering in thin nanowires can be damped strongly by coating the wire with a high-κ dielectric. This leads to an increase in the mobility of free charges inside the wire and can be used as a post-growth technique to improve the conductivity of thin nanowires. © *2007 American Institute of Physics*.
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Remarkable advances in crystal growth technology have recently enabled the fabrication of a variety of freestanding semiconductor nanostructures such as zero-dimensional (0D) nanocrystal quantum dots, 1D nanowires (NWs) and nanotubes, and 2D nanomembranes. Charge transport properties in such nanostructures are being intensively investigated, in the hope that they might find usage in electronic and optical devices in the future. These "bottom-up" nanostructures differ from the more extensively studied epitaxial nanostructures created by heterostructure bandgap engineering in one crucial aspect. The dielectric environment of epitaxial nanostructures is essentially the same as the semiconducting region (dielectric constant ϵ_s) where electrons and holes reside. However, for bottom-up nanostructures, the dielectric environment (ϵ_e) can be modified after growth. This feature offers a novel tool to engineer interactions between carriers and/or impurities mediated by the dielectric surrounding.

The effect of the dielectric environment on charge transport properties of bottom-up nanostructures has not received much attention as compared to its effect on optical properties.[1] Recent work[2] has shown that in 2D nanomembranes the electron mobility can be increased by one to two orders of magnitude by coating them with a high-κ dielectric material. The purpose of this work is to investigate the effect of the dielectric environment on electron transport in semiconductor nanowires. Semiconductor NWs can now be grown with diameters of a few nanometers, which is smaller than the thermal de Broglie wavelength of the carriers, while their lengths can exceed a few micrometers. At these length scales, the reduced density of states due to quantum confinement is expected to suppress scattering and lead to high carrier mobilities.[3] Recent experiments[4] have demonstrated improved carrier mobilities in Ge/Si nanowire field-effect transistors coated with high-κ (HfO_2) dielectrics.

In early work on carrier transport in 1D semiconductor nanowires,[5,6] the effect of dielectric mismatch on transport properties was not investigated. Vagner and Mösko showed in their treatment of a 1D electron gas confined in a *free-standing* 2D membrane that the dielectric mismatch leads to a large decrease in mobility.[7] In this article, we show that for 1D nanowires, the dielectric surrounding can be used to tune the electron mobility.

We consider an infinitely long semiconductor wire with a radius of few nanometers. To calculate the electron mobility in such a structure, we first investigate the effect of dielectric mismatch on the ionized-impurity (donor) scattering rate. For a positive impurity ion situated on the axis of the wire (see Fig. 1), the Fourier transform of the bare electrostatic potential inside the nanowire can be written as[8,9]

$$\tilde{V}^{\mathrm{Coul}}(\rho,k)=\frac{e}{4\pi^2\epsilon_s}\left[K_0(k\rho)+\frac{\pi\gamma}{2}e^{-2kR}I_0(k\rho)\right], \qquad (1)$$

where $\gamma=(\epsilon_s-\epsilon_e)/(\epsilon_s+\epsilon_e)$ is the dielectric mismatch factor, $I_0(\ldots)$ and $K_0(\ldots)$ are the zeroth order modified Bessel func-

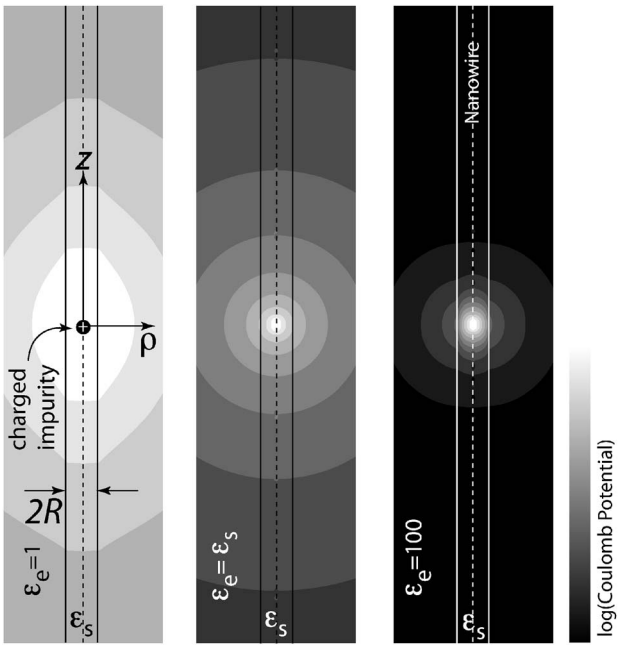

FIG. 1. Calculated Coulomb potential contours due to a point charge inside a nanowire for three different dielectric environments: $\epsilon_e=1,11,100$, $\epsilon_s=11$. The potential is strongly enhanced for freestanding wires ($\epsilon_e=1$), whereas it is strongly damped for a high-κ coating.

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tions, $k=k_z$ is the electron wavevector along the wire axis, ρ is the distance from the axis of the nanowire, R is radius of the nanowire, and e is the electron charge. In Eq. (1), the second term arises due to the dielectric mismatch ($\gamma \neq 0$) and is a very good approximation of the exact potential for $|kR| > 1/4$. Since Coulomb scattering is elastic, the momentum conservation rule allows only back scattering of carriers ($\vec{k} \rightarrow -\vec{k}$, $\vec{k}$ being the initial state) for transport in the first subband of the NW, and therefore results in a large momentum change ($q=2k$) in any elastic scattering process. So the assumption $|kR| > 1/4$ is justified.

The second term in Eq. (1) captures the dielectric mismatch effect. The Coulomb potential experienced by a carrier electron inside the wire is damped when $\epsilon_e \geq \epsilon_s$. For NWs with large radii, the transport properties in the nanowire should approach that of the bulk semiconductor; i.e., the dielectric mismatch should not affect the transport. This fact is captured in Eq. (1)—the mismatch term vanishes exponentially for large radii. In the long-wavelength limit, the real-space Coulomb potential experienced by an electron at $(\vec{\rho}, z)$, $|\vec{\rho}| < R$, $z \gg R$, is found from Eq. (1) to be $V^{\mathrm{Coul}}(z) \approx (e/4\pi\epsilon_e z)$, which indicates that Coulomb interaction within the wire is completely dominated by the *dielectric constant of the environment*.

Assuming that the electrons are confined in an infinite barrier potential, the electron energies are $E_n(k)=E_n+\hbar^2k^2/2m^\star$, where E_n is the ground-state energy of the nth 1D subband, and $m^\star$ is the electron effective mass. The corresponding envelope function is $\Psi_{n,\vec{k}}(\vec{\rho}, z) = \phi_n(\vec{\rho}) \cdot [\exp(ikz)/\sqrt{L}]$, where $\phi_n(\vec{\rho})$ is the radial part, $\hbar k$ is the longitudinal quasi-momentum, and L is the length of the nanowire. We chose E_1 as the reference of energy. For cylindrical nanowires, the radial part of the exact wave function takes the form of a Bessel function and can be used for a numerical evaluation of the scattering matrix elements. However, to illustrate the effect of the dielectric mismatch, for thin nanowires the ground state radial part of the envelope function can be approximated by $\phi_n(\vec{\rho}) \approx 1/\sqrt{\pi R^2}$. This leads to a slightly higher scattering rate than when the exact Bessel function is used, but (a) simplifies the treatment and (b) highlights the physics better. Thus, in this work a constant radial part of the electron wave function is used (see Ref. 6 for further justification). Then the matrix element for Coulomb scattering from state $|0,k_i\rangle \rightarrow |0,k_f\rangle$ is calculated to be

$$\tilde{v}^{\mathrm{Coul}}(q,R) = \frac{e^2}{2\pi\epsilon_s L x^2}\left[1 - xK_1(x) + \frac{\pi\gamma x e^{-2x}}{2} I_1(x)\right], \quad (2)$$

where $x=qR=|\vec{k}_i-\vec{k}_f|R$.

In addition to Coulomb impurity scattering, electrons in III-V NWs also suffer from longitudinal-optical (LO) phonon scattering at room temperature. LO phonon scattering is adequately modeled by 3D modes even for nanowires.[10] Taking the phonon wave vector to be $\vec{q}_{ph}=(\vec{Q}, q_z)$, $\vec{Q}=(q_x, q_y)$, the electron-phonon scattering matrix element can be written as[10]

$$\tilde{v}^{e-ph}(q,q_z,Q,R) = \sqrt{\frac{n_{ph}^{\pm} e^2 \hbar\omega_0}{2(Q^2+q_z^2)}\left(\frac{1}{\epsilon_s^\infty} - \frac{1}{\epsilon_s^0}\right)} \times \frac{2J_1(QR)}{QR}\delta_{q,\pm q_z}, \quad (3)$$

where ϵ_s^∞ (ϵ_s^0) is the high (zero) frequency dielectric constant of the semiconductor, $n_{ph}^- = [1+\exp(\hbar\omega_0/kT)]^{-1}$ and $n_{ph}^+ = (1+n_{ph}^-)\Theta[E_n(k)-\hbar\omega_0]$ stand for absorption and emission of a LO phonon of energy $\hbar\omega_0$, respectively ($\Theta[\ldots]$ is the Heaviside unit-step function), and $J_1(\ldots)$ is the Bessel function.

Using scattering matrix elements for the Coulomb and phonon scattering matrix defined in Eqs. (2) and (3), the scattering rate for the ith scattering mechanism is calculated as

$$\frac{1}{\tau_i(k)} = \frac{2\pi}{\hbar}\int \frac{dk'}{2\pi}\left|\frac{\tilde{v}^i}{\epsilon(q,0)}\right|^2 (1-\cos\theta) \times \delta(E_k - E_{k'} \pm \hbar\omega_0), \quad (4)$$

where $\pm\hbar\omega_0$ is required only for inelastic LO phonon scattering, and $\epsilon(q,0)$ is the screening factor in the static limit ($\omega \rightarrow 0$). The scattering rate is summed up over the final density of states and the Drude mobility is given by $\mu = e\langle\tau(T)\rangle/m^\star$, where $\langle\tau(T)\rangle$ is the ensemble-averaged scattering rate

$$\langle\tau(T)\rangle = \frac{\int_0^\infty dk k \tau_m(k)\left(-\frac{\partial f_0}{\partial k}\right)}{\int_0^\infty dk f_0(k)}. \quad (5)$$

Here $f_0(k)$ is the Fermi-Dirac distribution and $\tau_m(k)$ is the momentum relaxation time. The bare potential in NWs is screened due to the presence of free carriers. The quasi-1D screening function $\epsilon(q,0)$ can be calculated using the self-consistent procedure outlined by Lee and Spector;[11] we have included the effect of the dielectric mismatch to their screening theory. At low temperatures, the carriers contributing to transport are predominantly those at the Fermi level, and the momentum change upon scattering is $q \approx 2k_F$, where k_F is the Fermi wavevector. It is well known that the 1D screening function diverges for $q=2k_F$ at $T=0$ K. So, we have used Maldague's[12] prescription to remove the zero temperature singularity to obtain the finite temperature screening function as $\epsilon(q,0) = 1 + \Pi(q,R,T)/q^3$, where

$$\Pi(q,R,T) = \frac{\frac{1}{2} + I_1(v)\left[\frac{\pi\gamma e^{-2v}}{2} I_1(v) - K_1(v)\right]}{\pi R^2 a_B^\star} S(u), \quad (6)$$

where $v=2qR$, $u=\epsilon_F/k_BT$, and $a_B^\star$ is the effective Bohr-radius of the bulk semiconductor. $S(u)$ is a dimensionless integral defined in Ref. 6. Screening is strong for a low-κ dielectric coating around a NW with small radius. The effect of free-carrier screening is found to be negligibly small for NWs coated with a high-κ dielectric, as shown in Fig. 2. This can be understood from electrostatics: the electric field lines prefer to bunch in regions of high dielectric constant to lower the energy. Therefore, for a high-κ coating around a

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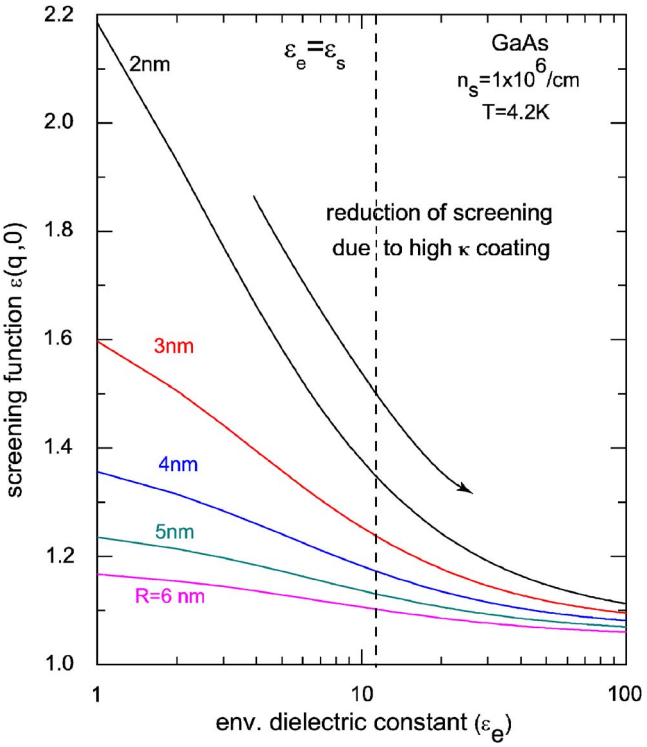

FIG. 2. (Color online) Screening function for different nanowire radii as a function of environmental dielectric constant: for low-κ dielectrics and small radii, screening is significant.

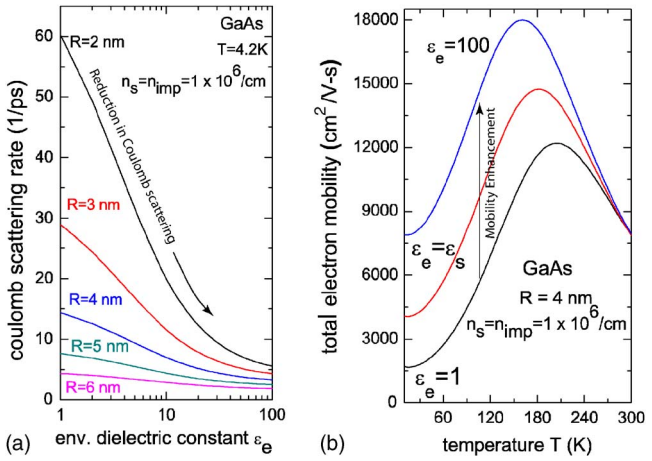

FIG. 3. (Color online) (a) Dependence of charged impurity scattering rate for various radii of NWs on the environmental dielectric constant. With increasing dielectric constant of the environment, the scattering rate decreases. (b) Electron mobility in a 4 nm GaAs NW as a function of temperatures for different dielectric environments.

thin NW, the field lines leak out into the surrounding and thus free-carrier screening becomes ineffective. For large NW radius, as expected, the dielectric mismatch has a very weak effect on screening (see Fig. 2).

For numerical evaluation of the effect of dielectric mismatch on transport, we assume a 1D electron density of $n_{1D}=10^6$ cm^{-1} and the ionized impurity density to be the same. For this density, the Fermi energy for a doped GaAs NW is $E_F=14$ meV. Then, to ensure that transport occurs in the first subband, the radius should be $R<20$ nm. At low temperatures, $E_F \gg k_B T$ and $q \approx 2k_F$, where k_F can be determined from the electron density ($k_F=\pi n_{1D}/2$). The calculated Coulomb scattering rates at $T=4.2$ K are shown in Fig. 3(a) for a GaAs NW with radii varying from 2 to 6 mm. For a 2 nm radius NW, the Coulomb scattering rate decreases from 60/ps to 6/ps when the dielectric constant in the environment is changed from 1 (air) to 100 (high-κ dielectric). With increasing radius, the Coulomb scattering rate becomes insensitive to the dielectric environment [see Eq. (2)].

For the calculation of temperature-dependent electron mobility, phonon scattering must be considered. Typical values for GaAs have been used ($\hbar\omega_0=36$ meV, $\epsilon_s^\infty=11\epsilon_0$, and $\epsilon_s^0=13\epsilon_0$). Phonon scattering rates are weakly dependent on the dielectric mismatch (γ) through the screening function. At low temperatures optical phonon scattering is negligible compared to the Coulomb scattering rate for our choice of impurity density. So, the carrier mobility in the nanowire is determined by Coulomb impurity scattering. Therefore, the electron mobility is strongly dependent on the dielectric environment, as shown in Fig. 3(b); for example, coating the GaAs NW with a high-κ dielectric can result in as much as four times enhancement in carrier mobility as compared to a freestanding nanowire due to the large damping of Coulomb scattering. At higher temperatures the LO phonon scattering rate increases and, at room temperature ($T=300$ K), LO phonon scattering dominates even for high impurity densities. As a result dielectric mismatch effect on the carrier mobility vanishes at room temperature. We point out here that in NWs made of elemental semiconductors such as Si or Ge, LO phonon scattering is weak and, for heavy doping, the dielectric mismatch induced enhancement in carrier mobility should persist up to room temperature. In comparison to semiconductor nanomembranes, the Coulomb scattering rate in wires is damped due to the reduced density of states near the Fermi energy, and therefore the drastic dielectric effect expected for nanomembranes[2] is not observed for doped III-V nanowires. Two questions that have not been addressed in this work are (a) the effect of charged surface states on nanowires and (b) the effect of surface roughness scattering. These are equally important questions since the presence of a large density of surface states on the nanowire will alter the electrostatic boundary conditions and hence lead to a different Coulomb potential. Similarly, surface roughness scattering can compete with Coulomb scattering at low temperatures and possibly even dominate for very thin wires with rough surface morphologies. These extensions to the core model investigated here will be presented in a more comprehensive later work.

In conclusion, we have investigated the effect of the dielectric environment on the electron mobility in semiconductor NWs. It is found that the Coulomb potential inside the nanowires can be tuned by the dielectric environment. Coating a thin NW with a high-κ dielectric will damp the Coulomb scattering and, if charged impurity scattering is the dominant scattering mechanism, mobility can indeed be improved. This is a novel technique for enhancing the mobility in nanostructures and is well suited for applications in field-effect transistor structures, where a high-κ dielectric affords better gate control, in addition to a higher mobility as shown in this work.

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