

Dielectric-environment mediated renormalization of many-body effects in a one-dimensional electron gas

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Relaxing the assumption of an “infinite and homogenous background,” the dielectric response function of one-dimensional semiconducting nanowires embedded in a dielectric environment is calculated. It is shown that a high- κ (higher than semiconductor dielectric constant) dielectric environment reduces the screening by the free carriers inside the nanostructure, whereas a low dielectric constant environment increases the Coulombic interaction between free carriers and enhances the strength of the screening function. In the long-wavelength limit, dielectric screening and collective excitations of electron gas are found to be strongly influenced by the environment. The behavior of the static dielectric function is particularly addressed at a specific wave vector $q = 2k_F$, a wave vector that ubiquitously appears in charge transport in nanostructures. It is shown that the exclusion of the dielectric mismatch effect in free-carrier screening results in an erroneous charged impurity scattering rate, particularly for nanowires embedded in low- κ dielectrics.

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I. INTRODUCTION

Low-dimensional structures such as semiconducting nanowires [one dimensional (1D)] are being investigated intensively for their potential applications in high-speed electronic and optical devices.¹ These nanowires can either be freestanding, or can be coated with different dielectric environments appropriate to device application. For example, in nanowire-based field-effect transistors (FETs), they are usually coated with high- κ dielectrics (HfO₂, ZrO₂, etc.)² for improved charge control and high electron mobility.³ On the other hand, for exciton-based devices, use of a low- κ (lower than the semiconductor dielectric constant ϵ_s) dielectric is beneficial as it enhances the excitonic binding energy.⁴ These advantages in electronic and optical properties stem from the fact that the Coulomb interaction between carriers and/or impurities inside the nanowires can be altered by altering the environment. This tunability of the carrier-carrier interaction by dielectric environment is expected to modify many-body effects such as dielectric screening by a one-dimensional electron gas (1DEG) inside the nanowire.

Dielectric screening by free carriers plays a crucial role in the transport quantities (conductivity, mobility, etc.) of a nanostructure. In a scattering event, the momentum-relaxation time (τ) strongly ($\tau \sim |\epsilon(q,0)|^{-2}$) depends on the free-electron screening inside the semiconductor. Hence an accurate knowledge of dielectric screening is necessary for a precise prediction of transport coefficients of a nanowire. The dielectric function of a semiconductor nanowire is composed of (i) ionic (ϵ^{ion}) and (ii) electronic (ϵ^{el}) contributions. ϵ^{ion} is an inherent property (crystal property) of semiconductors, while ϵ^{el} (commonly known as the screening function) depends on the magnitude of the electron-electron interaction inside a material. As the dielectric environment can alter the Coulomb potential inside a nanowire, it is expected that the dielectric environment will have a pronounced effect on the free-electron screening.⁵ Previous models⁶⁻⁹ for the dielectric function of 1DEG assume that the electron gas has an infinite homogenous background with a dielectric constant (ϵ_s) that is the same as the semiconductor. For a nanowire of few nm

radius, the “infinite background” approximation breaks down and at the nanowire/environment interface the “homogenous background” assumption fails. In this paper, assumptions are relaxed. By incorporating the dielectric mismatch factor at the nanowire/environment interface, a consistent theory of dielectric function is presented following the method of *self-consistent field*^{7,10,11} (also known as the random-phase approximation or RPA).

It is worthwhile to mention that the dielectric mismatch effect on the static screening is incorporated in recent numerical approaches (see Ref. 10) for Si/SiO₂ nanowires. The main concern of the work by Jin *et al.* was to investigate the surface roughness and the diameter-dependent electron mobility in nanowires mostly restricted to Si/SiO₂ nanowires. The effect of the dielectric environment on the free-carrier screening was not analyzed and hence the idea remained dormant so far. Here, following the general formalism developed in Ref. 10, and including the dielectric mismatch effect, an analytical expression of the dynamic dielectric function is evaluated. Both the static dielectric function and the collective excitations of 1DEGs in the long-wavelength limit are found to be solely determined by the dielectric environment. The importance of the modification of the static electronic screening by the dielectric environment is illustrated by calculating the screened ionized impurity scattering rates for nanowires embedded in both high- and low- κ dielectrics.

II. THEORETICAL FORMALISM

We consider an infinitely long semiconductor wire (dielectric constant ϵ_s) of a radius (R) of few nanometers embedded in a dielectric (dielectric constant ϵ_e) environment. To investigate the dielectric response of the electron gas inside the wire, we place an oscillating test charge at $(\mathbf{r}_0, z_0) = (0, 0)$ of density $n_0(r, t) = e\delta(\mathbf{r})e^{-i\omega t}$. This test charge creates an oscillating potential $V_0(r, z)e^{-i\omega t}$ in the nanowire and, in response to this perturbation, free electrons inside the nanowire rearrange themselves to screen the field. The resultant Hamiltonian of electrons confined in the wire is

$H = H_0 + V(\mathbf{r}, t)$, where $V(\mathbf{r}, t)$ is the self-consistent potential in response to the perturbation $V_0(\mathbf{r}, t)$. The unperturbed single-particle Hamiltonian $H_0 = \mathbf{p}^2/2m^* + V_{\text{con}}(r)$ satisfies the Schrödinger equation $H_0|n, k\rangle = \mathcal{E}_{n,k}|n, k\rangle$. Here m^* is the effective mass of electrons, k is the one-dimensional wave vector, $|n, k\rangle$ and $\mathcal{E}_{n,k}$ are the eigenvalues and eigenenergy of the unperturbed Hamiltonian, and $V_{\text{con}}(r)$ is the confinement potential for electrons inside the nanowire. Assuming electrons are confined in a infinite-barrier potential, the eigenenergies are $\mathcal{E}_{n,k} = \mathcal{E}_n + \hbar^2 k^2/2m^*$, where \mathcal{E}_n is the ground-state energy of the n th 1D subband and \hbar is the reduced Planck constant. The corresponding wave function is $\Psi_{n,k}(r, z) = \langle r|n, k\rangle = \phi_n(r)[\exp(ikz)/\sqrt{L}]$, where $\phi_n(r)$ is the radial part and L is the length of the nanowire. The dielectric function of an electron gas is defined by the relation¹²

$$V_{nn'} = \sum_{mm'} \epsilon_{nn', mm'}^{-1}(q, \omega) V_{mm'}^0, \quad (1)$$

where $\epsilon_{nn', mm'}^{-1}(q, \omega)$ is the four-dimensional dielectric matrix and $V_{ij}(V_{ij}^0) = \langle j, k + q|V(V_0)|i, k\rangle$ are the transition-matrix elements between states $|i, k\rangle$ and $|j, k + q\rangle$. Diagonal elements of the dielectric matrix represent the intrasubband polarization of the IDEG, whereas the off-diagonal terms result from intersubband transitions. In the size quantum limit (SQL) carriers are confined in the lowest ground state and intersubband separation is large, and the dielectric function becomes a scalar quantity.

The self-consistent potential contains both the original perturbation as well as the screened potential by the mobile charges, i.e., $V(\mathbf{r}, t) = V_0(\mathbf{r}, t) + V_{\text{sc}}(\mathbf{r}, t)$. For the evaluation of the dielectric response of a 1D electron gas, it is imperative to calculate the screening potential V_{sc} [see Eq. (1)]. The self-consistent potential $V(\mathbf{r}, t)$, upon acting on state $|n, k\rangle$, mixes it with other states such that wave function becomes $\Psi(r, t) = |n, k\rangle + \sum_{n', q} b_{k+q}(t)|n', k + q\rangle$. The coefficient $b_{k, k+q}(t)$ is given by time-dependent perturbation theory¹³

$$b_{k, k+q}(t) = \frac{V_{nn'}(q)e^{-i\omega t}}{\mathcal{E}_{n'}(k + q) - \mathcal{E}_n(k) - \hbar\omega}, \quad (2)$$

where $V_{nn'} = \langle n', k + q|V|n, k\rangle$ is the matrix element between state $|n, k\rangle$ and $|n', k + q\rangle$. The perturbation-induced charge density is $n^{\text{ind}}(r, t, z) = -2e \sum_{k, nn'} f_n^0(k)[|\Psi(r, t)|^2 - |\Psi_{n,k}(r, z)|^2]$, where, e is the charge of an electron and $f_n^0(k)$ denotes the equilibrium Fermi-Dirac occupation probability of a state $|n, k\rangle$ such that $2 \sum_{n, k} f_n^0(k) = n_{1d}$, n_{1d} being the equilibrium homogeneous unperturbed electron gas density. Assuming that the perturbation is weak enough such that the response is linear, and neglecting terms $b_{n, k+q}^2$ and higher orders, the induced charge density can be written as $n^{\text{ind}}(r, t) = -e \sum_{nn'} \phi_n(r)\phi_{n'}(r)V_{nn'}\mathcal{F}_{nn'}(q, \omega)e^{iqz}e^{i\omega t} + \text{c.c.}$, where c.c. denotes the complex conjugate and $\mathcal{F}_{nn}(q, \omega)$ is the polarization function¹³ (Lindhard function) obtained by summing the Feynman diagram of electron-electron interaction containing a single fermion loop,^{6,14}

$$\mathcal{F}_{nn'}(q, \omega) = \frac{2}{L} \sum_k \frac{f_n^0(k) - f_{n'}^0(k + q)}{\mathcal{E}_{n'}(k + q) - \mathcal{E}_n(k) - \hbar\omega}. \quad (3)$$

Note that the induced charge density has the same harmonic dependence as the self-consistent potential. The induced charge density is related to the screening potential by Poisson's equation $\nabla^2 V_{\text{sc}}(\mathbf{r}) = en^{\text{ind}}(\mathbf{r})/\epsilon_0\epsilon_s$, where ϵ_0 is the free-space permittivity. Expressing screening potential in Fourier components $V_{\text{sc}}(r, z) = \sum_{-\infty}^{\infty} v_{\text{sc}}(r, q)e^{iqz}$, where $q = k' - k$, one obtains the differential equation for the screening potential

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dv_{\text{sc}}}{dr} \right) - q^2 v_{\text{sc}} = \begin{cases} en^{\text{ind}}(r)/\epsilon_0\epsilon_s, & r \leq R, \\ 0, & r \geq R. \end{cases} \quad (4)$$

The Green's function appropriate to the above differential equation with dielectric mismatch effect is^{3,10,15}

$$G(r, r', q) = \frac{1}{\pi} \left[\underbrace{I_0(q \cdot r_{<}) K_0(q r_{>})}_{g^{\text{inhom}}(r, r')} + \underbrace{\mathcal{U}(qR) I_0(qR) K_0(q r')}_{g^{\text{hom}}(r, r')} \right], \quad (5)$$

$$\mathcal{U}(x) = \frac{(\epsilon_s - \epsilon_e) K_0(x) K_1(x)}{\epsilon_e I_0(x) K_1(x) + \epsilon_s I_1(x) K_0(x)}$$

where $g^{\text{hom}}(g^{\text{inhom}})(r, r')$ is the homogenous (inhomogenous) part of the Green's function, $r_{<(>)} = \min(\max)[r, r']$, and $I_n(\dots)$ and $K_n(\dots)$ are the n th-order modified Bessel functions. For large x ($x > |n^2 - 1|$), $I_n(x) \approx e^x/\sqrt{2\pi x}$, $K_n(x) \approx e^{-x}\sqrt{2\pi/x}$, and the function $\mathcal{U}(qR) \rightarrow (\pi\gamma/2)e^{-2qR}$, where $\gamma = (\epsilon_s - \epsilon_e)/(\epsilon_s + \epsilon_e)$ is the dielectric mismatch factor. The tunability of the strength of the Green's function arises through its dependence on γ , which enhances (reduces) the strength for $\epsilon_s > \epsilon_e$ ($\epsilon_s < \epsilon_e$). For an infinite homogeneous environment ($\epsilon_e = \epsilon_s$), $\gamma = 0$, and the Green's function is independent of the dielectric environment. Using the above Green's function, the induced potential inside the nanowire can be written as $v_{\text{sc}}(r, q) = e/4\pi\epsilon_0\epsilon_s \int_0^R G(r, r', q) n^{\text{ind}}(r') r' dr$.¹⁶ In the size quantum limit (SQL), the nanowire is thin ($R < \lambda_{\text{dB}}$, where λ_{dB} is the de Broglie wavelength of an electron) and only the lowest subband is populated. Moreover, for a thin nanowire, the intersubband separation energy is large ($\Delta\mathcal{E}_n \propto 1/R^2$) such that the intersubband transition can be neglected ($n = n' = 1$). In such a scenario, the dielectric matrix becomes scalar, i.e., $\epsilon_{nn'}(q, \omega) \rightarrow \epsilon_{11}(q, \omega)$. Assuming $\phi_{n=1}(r) \approx 1/\sqrt{\pi R^2}$, the dynamic dielectric function of an IDEG at temperature $T = 0$ is¹⁷

$$\epsilon_{1d}(q, \omega, \mathcal{E}_F) = 1 - \frac{e}{4\pi\epsilon_0\epsilon_s V_{11}} \int_0^R \phi_1^2(r) r \times \int_0^R G(r, r') n^{\text{ind}}(r') r' dr' dr$$

$$= 1 + \frac{1}{\pi a_B^* R^2} \frac{F(x)}{q^3} \ln \left| \frac{(q + 2k_F)^2 - \left(\frac{2m^*\omega}{\hbar q}\right)^2}{(q - 2k_F)^2 - \left(\frac{2m^*\omega}{\hbar q}\right)^2} \right|, \quad (6)$$

where $x = qR$ is a dimensionless quantity, $F(x) = \frac{1}{2} + I_1(x)[\mathcal{U}(x)I_1(x) - K_1(x)]$, $a_B^* = 4\pi\epsilon_0\epsilon_s\hbar^2/m^*e^2$ is the effective bulk Bohr radius, $k_F = \pi n_{1d}/2$ is the Fermi wave vector, and $\mathcal{E}_F = \hbar^2 k_F^2/(2m^*)$ is the corresponding Fermi energy. The logarithmic term in Eq. (6) is results from the Lindhard function $\mathcal{F}_{11}(q, \omega)$, which has been evaluated analytically in the SQL.⁶ In the context of charge transport inside the nanowire, the static part of the dielectric function $\epsilon_{1d}(q, \omega = 0)$ is relevant. In the long-wavelength ($q \ll 2k_F$) limit, the static

dielectric function $\epsilon_{1d}(q,0)$ for a thin nanowire ($qR \rightarrow 0$) becomes

$$\epsilon_{1d}(q,0) = 1 - \frac{e^2}{2\pi\epsilon_0\epsilon_e} [\ln(qR)] \mathcal{D}_{1d}(\mathcal{E}_F), \quad (7)$$

where $\mathcal{D}_{1d}(\mathcal{E}_F) = (1/\pi\hbar)\sqrt{2m^*/\mathcal{E}_F}$ is the 1D density of states per unit length at Fermi energy \mathcal{E}_F . In sharp contrast to previous models,¹² the dielectric constant of the environment (ϵ_e), instead of the semiconductor itself (ϵ_s), determines the long-wavelength behavior of the static dielectric function.

For a large momentum ($q \gg 2k_F$), $\epsilon_{1d}(q,0) \rightarrow 1$ as the second term of Eq. (6) falls off rapidly (q^{-5}) with q . For a degenerate 1DEG in SQL, only backscattering is allowed, which leads to a momentum transfer $q = 2k_F$ in any intrasubband elastic scattering process. As a result, $\epsilon_{1d}(q = 2k_F, 0)$ plays an important role in momentum relaxation rate calculation. In the static limit ($\omega = 0$), the dielectric function $\epsilon_{1d}(q,0)$ at $T = 0$ is singular for $q = 2k_F$. This divergence is related to Peierl's instability, which is a characteristic signature of a 1DEG. At finite temperature, smearing of the Fermi function removes this singularity. The static dielectric function at $T \neq 0$ is given by Maldague's prescription¹⁸

$$\epsilon_{1d}^T(q,0) = \int_0^\infty d\mathcal{E} \epsilon_{1d}(q,0,\mathcal{E}) \left[4k_B T \cosh^2 \left[\frac{\mathcal{E} - \mathcal{E}_F}{2k_B T} \right] \right]^{-1}. \quad (8)$$

III. RESULTS AND DISCUSSIONS

Figure 1(a) shows the static dielectric function of a GaAs nanowire at $q = 2k_F$ with a nanowire radius R for three different dielectric media. Note that even negligible smearing of Fermi distribution at $T = 4.2$ K is enough to remove the divergence at $q = 2k_F$. For coated nanowires with $\epsilon_e > \epsilon_s$, dielectric screening is strongly reduced as shown in Fig. 2(b). At large radius ($R \gg 1/4k_F$), the nanowire tends to the bulk structure and the dielectric mismatch effect on the screening function vanishes. With increasing carrier density, dielectric

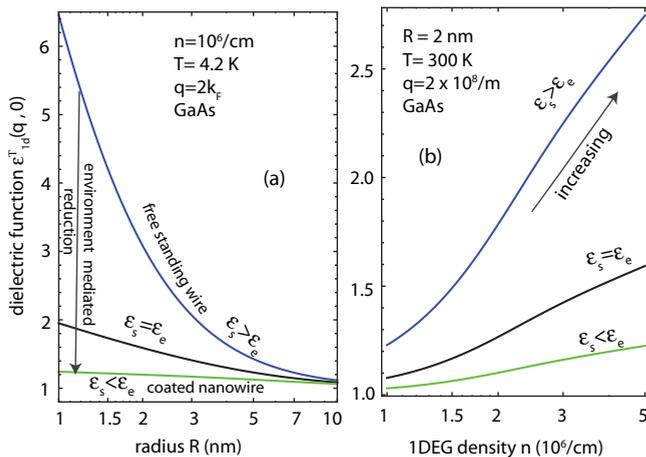


FIG. 1. (Color online) Dielectric function of a nanowire (a) with nanowire radius (R) and (b) as a function of carrier density (n) for three different dielectric environments of $\epsilon_e = 1$ (upper branch), $\epsilon_e = \epsilon_s = 13$ (middle), and $\epsilon_e = 100$ (lower branch).

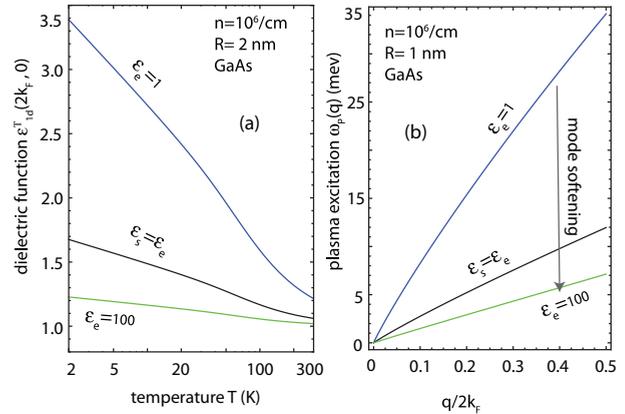


FIG. 2. (Color online) (a) Dielectric function of a nanowire with temperature (T) and (b) plasma frequency of an 1DEG with wave vector (q) for three different dielectric environments.

screening inside the nanowire increases [see Fig. 1(b)], maintaining the effect of the dielectric environment. At higher carrier densities, more than one subband is populated and the intersubband contribution to the total dielectric function should be taken into account for a complete description of free-electron screening inside the nanowire. With increasing temperature, thermal fluctuation reduces the free-electron screening inside the nanowire, and the effect of environmental dielectric on the screening function is partially washed away [see Fig. 2(a)].

As the dynamic ($\omega \neq 0$) dielectric function $\epsilon_{1d}(q,\omega)$ contains the dielectric mismatch factor, collective excitations of the 1DEG are also expected to depend on the dielectric environment. Collective excitation of an electron gas is defined as the pole of the full dynamic dielectric function, i.e., by $\epsilon_{1d}(q,\omega_p) = 0$, where ω_p is the plasma frequency of the electron gas. Figure 2(b) shows the plasma dispersion of intrasubband collective excitation of a thin nanowire ($R = 2$ nm) for different dielectric environments. For $q < 1/2R$, the dielectric environment has a finite effect on the collective excitation frequency of 1DEG. The softening of plasma frequency with a high- ϵ_e dielectric environment is the consequence of the reduction of the Coulomb interaction between electrons and the positive background, which acts as a restoration force of the collective oscillation of the electron gas. For small q , the frequency of collective excitations goes to zero for all of the dielectric environment following the relation $\omega_p(q) \approx \omega_0 q \sqrt{-\ln(qR)}$, where $\omega_0 = \sqrt{n_{1d}e^2/(4\pi\epsilon_0\epsilon_e m^*)}$. Note the explicit appearance of ϵ_e in ω_0 highlights the role of the environment in the collective excitation of 1DEG inside the wire.

A typical example where the static dielectric function plays a crucial role is the determination of the charged impurity scattering rate in semiconductor nanostructures. Figure 3(a) shows the screened Coulomb scattering rates at low temperature with (solid lines) and without (dashed lines) accounting for the dielectric mismatch effect in free-carrier screening for an impurity point charge e located on the axis of the nanowire. Here, we use the Coulomb potential derived in Ref. 3. Note that the exclusion of the dielectric mismatch effect in the screening underestimates (overestimates) the

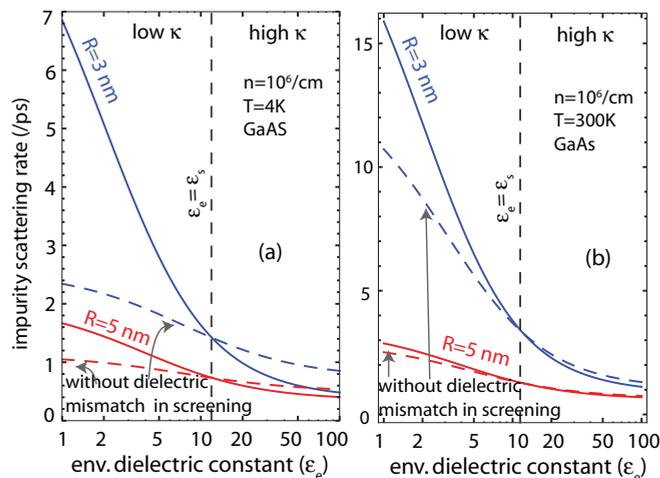


FIG. 3. (Color online) Screened Coulomb scattering rate with (solid) and without (dashed) incorporating the dielectric mismatch in static screening at (a) low temperature, and at (b) room temperature as a function of dielectric constant of the environment. Here we assumed an impurity density $n_{\text{imp}} = 2.5 \times 10^5/\text{cm}$.

scattering rate [see Fig. 3(a)] for the low- κ (high- κ) dielectric medium surrounding the thin ($R \leq 5$ nm) nanowires. At room temperature, weak free-carrier screening results in a higher scattering rate [see Fig. 3(b) as compared to Fig. 3(a)]. At room temperature, the dielectric mismatch effect on the free-carrier screening can be neglected for high- κ dielectric environments, although for low- κ environments, inclusion of the dielectric mismatch effect in screening is necessary for an accurate evaluation [see Fig. 3(b)] of scattering rates.

The length scale at which the dielectric environment plays an important role can be determined by investigating the behavior of $\mathcal{U}(qR)$. For large qR , $\mathcal{U}(qR) \sim e^{-4k_F R}$. Hence, for $R \gg 1/(4k_F)$, $\mathcal{U}(qR)$ becomes negligible and the dielectric effect vanishes. For numerical estimates, at a carrier density

$n_{1d} = 10^6/\text{cm}$, the dielectric effect vanishes for $R \gg 2$ nm, whereas at a lower density ($n_{1d} = 10^5/\text{cm}$) the environmental effect on the quantum screening function persists for a wire radius of up to $R \approx 20$ nm.

We have assumed an infinite confining potential for electron inside the wire. Relaxing this assumption will result in electron mass enhancement due to leaking of the wave function into the barrier. For high- κ oxides the typical barrier height is ~ 1 eV, for which a nominal increase in electron mass can be neglected.¹⁹ The assumption of a constant radial part of the wave function is justified for thin nanowires. Choosing a different form for the radial part will change the absolute value of the screening function for thick (for large R the dielectric-environment effect reduces anyway) wires, keeping the relative effect of environments unchanged.

IV. CONCLUSION

In conclusion, we have shown that the free-electron screening inside a nanowire depends on the environment surrounding it. For a nanowire coated with a high- κ dielectric, Coulomb perturbation inside the nanowire is poorly screened as compared to a freestanding nanowire. It is shown that both the static dielectric function and the plasma dispersion in the long-wavelength limit gets modified by the environment. The length scale at which the environment has a substantial effect on the electron gas inside the nanowire was identified. The results are analytical and will be useful for accurate predictions of transport coefficients in nanowire-based electronic devices.

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⁵One such example is the dielectric-environment mediated free-electron screening in graphene, where an average dielectric constant of graphene $\epsilon_{\text{gr}}^{\text{avg}} = (\epsilon_e^t + \epsilon_e^b)/2$ is used in the Thomas-Fermi screening function. Here $\epsilon_e^t(\epsilon_e^b)$ is the dielectric constant of the top (bottom) environment of graphene and the crystal property of the atomically thin (monolayer 0.3 nm) graphene is neglected. For a nanowire with a radius of a few nm, the crystal property of the semiconductor cannot be neglected and a rigorous model containing both ϵ_e and ϵ_s is necessary.

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