

Radiated fields by polygonal core-shell nanowires

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ABSTRACT

We calculate the electromagnetic field radiated by tubular nanowires with prismatic geometry and infinite length. The polygonal geometry has implications on the electronic localization; the lowest energy states are localized at the edges of the prism and are separated by a considerable energy gap from the states localized on the facets. This localization can be controlled with external electric or magnetic fields. In particular, by applying a magnetic field transverse to the wire the states may become localized on the lateral regions of the shell, relatively to the direction of the field, leading to channels of opposite currents. Because of the prismatic geometry of the nanowire the current distribution, and hence the radiated electromagnetic field, have an anisotropic structure, which can be modified by the external fields. In this work we study hexagonal, square and triangular nanowires.

Keywords: core-shell nanowires, electronic transport, radiation.

1. INTRODUCTION

Core-shell nanowires made of semiconductor materials, with diameters between a few tens and a few hundred nm, have recently attracted great interest as a result of their rich electronic properties, related both to transport and optics. Typically, such nanowires are fabricated by the bottom-up method and have polygonal cross sections, most often hexagonal [1, 2]. Still, other polygonal shapes are possible, like square [3] or triangular [4, 5, 6]. Interestingly, in such structures the shell can be conductive and the core can be insulating, such that one obtains a tubular conductor with a prismatic geometry. In this geometry the electrons with low energies, situated within the shell, tend to be localized along the prism edges, as the corners of the cross section act like local quantum wells with a binding effect [7, 8, 9]. In principle, for a polygon with N corners, this group consist of $2N$ states, where the factor 2 accounts for the spin. For thin shells and sharp angles these states are nearly degenerate. Next on the energy scale there is another group of $2N$ states localized on the prism facets. Depending on the geometric parameters of the shell the two groups of states can be separated by a remarkably large energy interval, possibly of tens of meV, or even more for the triangular case [10, 11].

In this work we study theoretically the electromagnetic fields radiated by such prismatic shells. We obtain numerically the quantum mechanical states and calculate the current along the nanowires considering a time-dependant harmonic voltage bias. We discuss the implication of the corner states on the radiated field for the three different geometries. We also study the controllability of the filed distribution with electric and magnetic fields external to the nanowire, which break the spatial symmetry of the charge and current distributions within the shell.

2. THE MODEL

We focus on a system of non-interacting electrons confined in an infinite nanowire with polygonal cross section. Our approach to model the polygonal cross section begins with a circular ring, situated in the plane (x, y) , described by discretized polar coordinates [12], on which we superimpose polygonal constraints and retain the points situated within the resulting shell. We assume free particle scattering along the longitudinal direction z . The Hamiltonian of the system can be expressed as:

$$H = \frac{(-i\hbar\nabla + e\mathbf{A})^2}{2m_{\text{eff}}} - e\mathbf{E} \cdot \mathbf{r} - g_{\text{eff}} \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}. \quad (1)$$

We denote by $\mathbf{E} = (E_x, E_y, 0)$ and $\mathbf{B} = (B_x, B_y, 0)$ the transverse electric and magnetic fields, respectively, which can be chosen at any angle relatively to the shell edges, and by \mathbf{A} the vector potential associated with the magnetic field. Also, $\mathbf{r} = (x, y, z)$ is the position vector within the shell volume, e is the electron charge, m_{eff} and g_{eff} are the effective electron mass and g-factor in the shell material, μ_B is Bohr's magneton, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ stands for the spin related Pauli matrices.

We calculate the eigenstates of the Hamiltonian (1) numerically, in two steps: first for $\mathbf{B} = 0$, to obtain the eigenvectors of the transverse motion in the position representation, $|a\rangle$, where $a = 1, 2, 3, \dots$, on a lattice with 6000-10000 points, depending on the geometry. Then we use the first $2N$ modes, N being the number of shell corners, we form the basis set $|aks\rangle$, where k is the wave vector corresponding to the longitudinal motion, and

$s = \pm 1$ is the spin label, and we diagonalize the total Hamiltonian for $\mathbf{B} \neq 0$, for a discretized series of k values, to obtain its eigenvalues E_{mks} ($m = 1, 2, 3, \dots$), and its eigenvectors $|mks\rangle$ expanded in the basis $|aks\rangle$.

This procedure gives us the states with the lowest energies, localized along the edges or of the prismatic shells. Using them we compute charge density ρ and the current density \mathbf{J} inside the shell as:

$$\rho(\mathbf{r}) = e \sum_{mks} \mathcal{F} \left(\frac{E_{mks} - \mu}{k_B T} \right) [|\langle \mathbf{r} | mks \rangle|^2 - en_d], \quad \mathbf{J}(\mathbf{r}) = \sum_{mks} \mathcal{F} \left(\frac{E_{mks} - \mu}{k_B T} \right) \langle mks | \mathbf{j}(\mathbf{r} - \mathbf{r}_0) | mks \rangle, \quad (2)$$

where $\mathcal{F}(u) = 1/[\exp(u) + 1]$ is the Fermi function with $u = (E_{mks} - \mu)/k_B T$, μ stands for the chemical potential, T the temperature, and k_B Boltzmann's constant. The second term of the charge density represents the background of ionized donors of density n_d . The operator $\mathbf{j}(\mathbf{r}, \mathbf{r}_0) = e[\delta(\mathbf{r} - \mathbf{r}_0)\mathbf{v} + \mathbf{v}\delta(\mathbf{r} - \mathbf{r}_0)]/2$ describes the contribution at spatial point \mathbf{r} from an electron situated at \mathbf{r}_0 which moves with the velocity described by the operator $\mathbf{v}(\mathbf{r}_0) = i[H, \mathbf{r}_0]/\hbar$.

Obviously, in equilibrium, i.e. when no longitudinal voltage is applied on the nanowire, the total current is zero; the current corresponding to the electrons moving with positive velocity compensates the current of those moving with negative velocity in the z direction. In order to generate a non-zero total current we simulate a voltage bias by creating an imbalance between the states with positive and negative velocity, i.e. with $\partial E_{mks}/\partial k > 0$, and $\partial E_{mks}/\partial k < 0$, respectively [13]. To implement it we consider two different chemical potentials, μ_+ and μ_- , associated with positive and negative velocities, variable in time in a harmonic manner, $\mu_{\pm} = \mu \pm V \sin(\omega t)$, i.e. with frequency ω and amplitude $2V$, where the static chemical potential μ is determined by the carrier density at equilibrium. Using Eqs. (2) we compute the time dependent charge and current densities in the tubular shell, and then we calculate the radiated scalar and vector potentials outside the nanowire, as

$$\Phi_{rad}(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}', \quad \mathbf{A}_{rad}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}', \quad (3)$$

where the integration is performed within the shell domain, and ϵ_0, μ_0 are the vacuum constants. Finally we obtain the radiated electric and magnetic fields using the Maxwell equations:

$$\mathbf{E}_{rad} = -\nabla\Phi_{rad} - \frac{\partial \mathbf{A}_{rad}}{\partial t}, \quad \mathbf{B}_{rad} = \nabla \times \mathbf{A}_{rad}. \quad (4)$$

In our present approach we neglect the retardation effects, since the speed of light can be considered infinite at the nanometric scale. In addition we consider an arbitrary (unspecified) frequency ω , but in principle sufficiently low to prevent strong damping. Our main goal is to show qualitatively the fingerprint of the tubular prismatic geometry on the spatial structure of the radiated field, and in particular the combined effect of localization and external fields.

3. RESULTS

In this section we show qualitatively some examples of radiated field configurations for the three polygonal geometries: hexagonal, square, and triangular. For simplicity we represent the radiated field by the corresponding magnetic component. We use InAs bulk parameters for the shell: $m_{\text{eff}} = 0.023m_e$ and $g_{\text{eff}} = -14.9$. In all cases the external radius of the polygonal shell is $R_{\text{ext}} = 50$ nm and the thickness of the facets is $t = 10$ nm. Also, the amplitude of the AC voltage bias used is fixed to $2V = 5$ meV.

In Figures 1, 2, and 3 we first show, for each geometry, the energy spectra for the symmetric shells. In Panels (a) we indicate with blue lines the corner states, with red lines the side states, and the energy interval between them with Δ . We assume that the chemical potential is sufficiently low (or, equivalently, the electron density is low), such that only the corner states are populated. With this condition the anisotropy related to the internal structure of the nanowire is maximal. As mentioned before, we obtain twelve corner states for the hexagonal, eight for the square, and six for the triangular geometries. Because of the spin and rotational symmetries these states can be two or four-fold degenerate, such that multiple blue (and also red) lines overlap in Panels (a) of each figure.

Next, we show the current distributions and the radiated fields for three situations: first the nanowires with the polygonal symmetric distribution of electrons, and then in the presence of the transverse electric or magnetic fields. If the polygonal shell is perfectly symmetric the electrons are equally distributed between the corners. In this case, in the presence of a chemical potential bias, currents are running in parallel along the prism edges, as shown in Panels (b). The radiated electromagnetic field from each edge is similar to the one created by a line of current. The total field is thus a superposition of the N edge currents, with the spatial symmetry of the prismatic shell.

An external transverse (static) electric field breaks this spatial symmetry of the charge distribution by pushing the electrons laterally, and allowing for the controllability of the localization. This perturbation leads to a different

structure of the radiated field in the vicinity of the nanowire, as shown in Panels (c). We notice that the anisotropy of the radiated field increases for the square and furthermore for the triangular shell. The Panels (b) and (c) correspond to the instant in time when the voltage bias is maximized, i.e. $\mu_+ - \mu_- = 2V$.

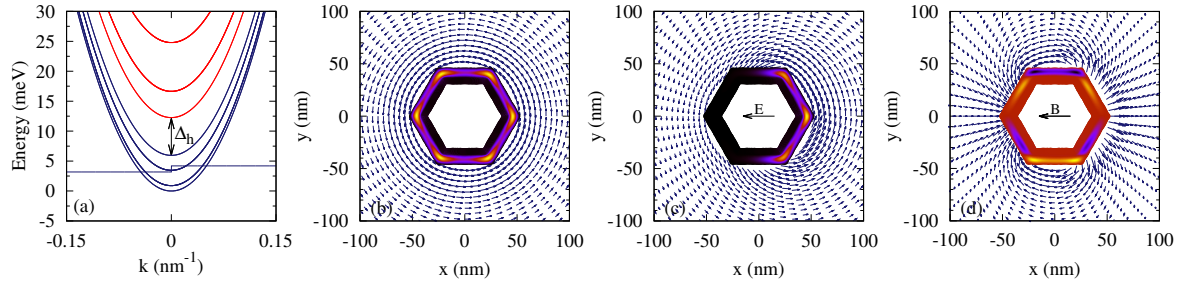


Figure 1: *Hexagonal shell. (a) Energy spectrum in the absence of external fields. The blue curves correspond to the corner-localized states and the red ones to the side-localized states. The energy separation between them is $\Delta_h = 6.5$ meV. The horizontal lines indicate the biased chemical potential at maximum amplitude $2V = 5$ meV. (b) The current distribution and the radiated field in the absence of external fields. The current distribution inside the shell is shown on a color scale, with the yellow and purple colors corresponding to electrons propagating in the positive and negative z direction, respectively, and with black color corresponding to regions with vanishing electron density. The radiated magnetic field outside the nanowire is represented with arrows. (c) The current distribution and the radiated magnetic field in the presence of an external electric field $E = 10$ $\mu\text{V}/\text{nm}$. (d) The current distribution and the radiated magnetic field in the presence of an external magnetic field $B = 1$ T.*

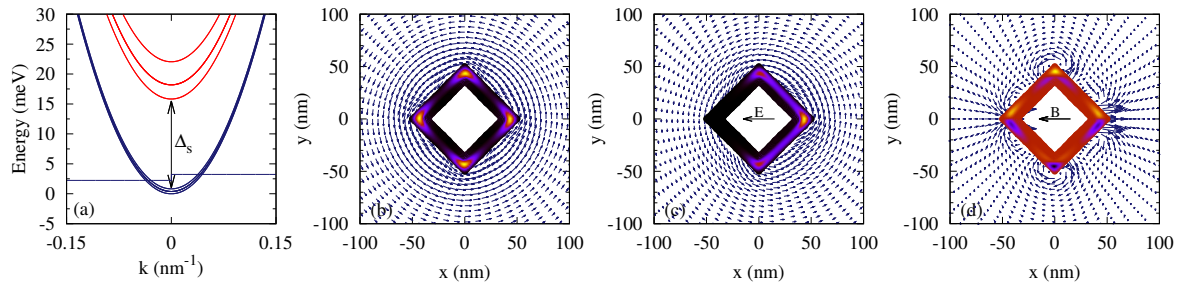


Figure 2: *Similar to Fig. 1, but for a square shell. In this case $\Delta_s = 14.6$ meV.*

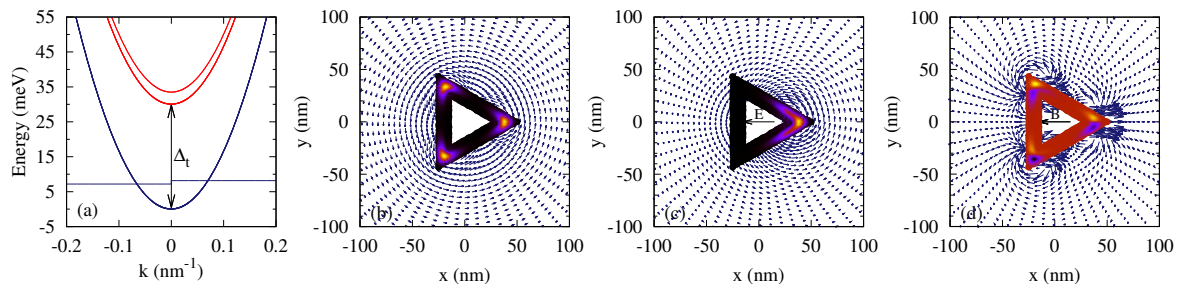


Figure 3: *Similar to Figs. 1 and 2, but now for a triangular shell, with $\Delta_t = 27.1$ meV.*

A much more interesting situation occurs when a magnetic field is applied perpendicular to the nanowire. In Panels (d) we show the case when it is applied along a certain symmetry axis of the prismatic shell. In this situation the corner localization coexists with the localization induced by the magnetic field. The magnetic localization is determined by the motion of the electrons along the nanowire and can lead to the formation of local Landau states in the regions where the radial component of the magnetic field is locally constant, and of snaking states in the regions where it changes sign. The density of electrons tends to increase around the snaking states [14]. Consequently, we obtain channels of current traveling in opposite directions. These channels can also be considered as large loops of current along the nanowire length driven by the Lorentz force. To illustrate this fact we selected the instant in time when the chemical potential bias is zero and there is no net current through the nanowire, each current

channel being compensated by its pair. Remarkably, the paired channels can be situated on opposite sides of the shell, but also within the same corner. In the hexagonal case the external magnetic field induces three loops: one along the facets parallel to the magnetic field, and two more in the other facets, Fig. 1(d). In the case shown for the square geometry we obtain current channels only in the corner areas: snaking states in the corners lateral to the direction of the field and local Landau states in the other two corners. In the example shown for the triangular shell, Fig. 3(d), where the binding effect is the strongest, the electrons form three loops: two of them within the facet perpendicular to the magnetic field and one in the opposite corner, all of Landau type.

Thus, in the presence of a transverse magnetic field, the radiated field can be much richer in structure than in the previous cases. The magnetic field radiated can be highly anisotropic near the shell, especially for the square and triangular geometries, and resembles the field created by a magnetic dipole.

4. CONCLUSIONS

We discussed the magnetic component of the electromagnetic field radiated by polygonal core-shell nanowires exposed to transverse electric or magnetic fields, which allow to control the localization of electrons. We showed that the internal geometry of the nanowire has implications on the configuration of the radiated field. In particular, an external transverse magnetic field induces longitudinal channels of electrons traveling in opposite directions, which may lead to a highly anisotropic radiated field.

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