Disorder-induced enhancement of conductance in doped nanowires*

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A new mechanism is proposed to explain the enhancement of conductance in doped nanowires. It is shown that the anomalous enhancement of conductance is due to surface doping. The conductance in doped nanowires increases with dopant concentration, which is qualitatively consistent with the existing experimental results. In addition, the I–V curves are linear and thus suggest that the metal electrodes make ohmic contacts to the shell-doped nanowires. The electric current increases with wire diameter (D) and decreases exponentially with wire length (L). Therefore, the doped nanowires have potential application in nanoscale electronic and optoelectronic devices.

Keywords: conductance, nanowires

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1. Introduction

Semiconductor nanowires have attracted much attention in recent years, due to potential applications,[1−17] such as optoelectronics,[1−3] nanoscale electronics,[3−12] sensors,[13,14] and spintronics,[15] etc. More recently, electrical transport measurements showed that the conductivity of the semiconductor nanowires can be increased by modulating doping.[18−21] For instance, Cui *et al.*[18] found that it is possible to incorporate high boron or phosphorus impurity atoms in the Si nanowires and to approach the metallic regime. Yu *et al.*[19] reported that the conductance of highly gold- and zinc-doped silicon nanowires is substantially larger than expected. Ma *et al.*[20] showed that electrical conductivity has been clearly enhanced in the B-doped silicon nanowires. Huo *el al.*[21] observed that the conductance of Cu-doped ZnTe nanowires can be increased by about three orders of magnitude. These experimental results are in sharp contradiction to the Anderson disorder picture that any mount of disorder in one-dimensional systems results in carrier localisation, and the larger the disorder, the stronger the localisation.[22] Therefore, the intrinsic mechanism of electric transport in doped nanowires deserves our consideration.

A field-effect transistor based on a shell-doped nanowire is shown schematically in left panel of Fig. 1. By tight-binding theory, interestingly, the numerical results of the shell-doped nanowire model not only illuminate some of the unusual experimental results discussed above but also suggest general principles for understanding and control of transport properties in nanowires. In experiment, the doped nanowire is connected to two electronic reservoirs by lead contacts. Similarly, the whole model system adopted in this letter consists of a central sample (a shell-doped nanowire) with a finite length and two semi-infinite leads (left and right), in which the two semi-infinite leads are assumed to be made of perfect nanowires. Before doping, the surface disorder is considered to exist on the surface of nanowires due to surface reconstruction. Based on Anderson-type tight-binding Hamiltonian, the electric currents and conductance of the shell-doped nanowires are calculated. It can be seen that the heavily shell-doped nanowires approach to a metallic regime with the strength of disorder. The electric current increases with wire diameter (D) and decreases exponentially with wire length (L). These results can help understanding the effects of fabrication, processing, and measurement-induced surface contamination on transport properties.

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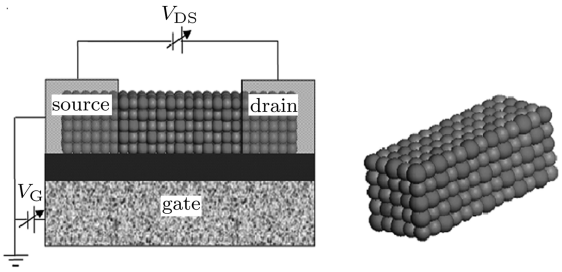


Fig. 1. Schematic cross section of the device (left). Schematic illustration of a nanowire with surface disorder induced by shell-doping (right).

2. Model and method

As shown in the right panel of Fig. 1, the dopant atoms are distributed within a few layers in the shell region of a nanowire. The cross section of the wire is a square lattice of size $D^2 = na \times na$, where a is the lattice constant. The length of the nanowire is $L = pa$ with $p >> n$. The tight-binding Hamiltonian obtained by considering non-interacting electrons is given by $H = \sum_i \varepsilon_i c_i^+ c_i + \sum_{i,j} V(i,j) c_i^+ c_j$, with on-site energy ε_i, where i labels the coordinates of the sites in the lattice. The hopping integral $V(i,j) = t = 1$ eV is restricted to the nearest neighbours of a site. In the absence of doping, there exists disorder on the surface of nanowires, due to surface reconstruction. In the presence of doping, the on-site energy ε_i takes random values distributed within an interval $[-\xi, \xi]$ for the shell region, with ξ describing the degree of the shell disorder introduced not only by dopant atoms but also surface reconstruction. To obtain good statistics, we have used up to 200 different configurations in this paper. By using a recursive green function method,[23] the transmission coefficient between the left and right leads can be calculated by $T(E) = \mathrm{Tr}(\Gamma_\mathrm{L} G^r \Gamma_\mathrm{R} G^a)$. Based on generalised Landauer approach, the tunneling current at a finite temperature is given by $I = (2e/\hbar) \int \mathrm{d}E T(E) [f_1(E - u_\mathrm{L}) - f_2(E - u_\mathrm{R})]$,[24,25] where the factor 2 accounts for degeneracy, $f_1(E - u_\mathrm{L})$ and $f_2(E - u_\mathrm{R})$ are the Fermi energy functions of the waves incident from the two electrodes to the device. Note that in the present work, we calculate only the phase-coherent transmission coefficient. The effect of electron–phonon interaction is neglected and the temperature dependence is only via the Fermi factors of electrons.

3. Calculations and discussion

Figure 2 shows the calculated I–V curves of the perfect nanowire with different potential barriers and/or wells $U = 0$, $\pm 0.2t$, $\pm 0.5t$, respectively. Two distinct characters can be seen clearly from Fig. 2. It is shown that in the absence of the applied gate voltage, a small nonlinearity is observed in the intrinsic nanowire ($\xi = 0$), which indicates that this contact is slightly nonohmic. The conductance is obtained to be about 19.5 $2e^2/h$. By increasing the applied gate voltage, the current is quenched to zero in the range from $-U$ to U. As shown in Fig. 2, the current begins to increase only when the bias voltage exceeds the threshold voltage. These results indicate that the perfect nanowires show rectifying effect. In the perfect nanowire, the origin of the rectifier is attributed to the symmetry transmission curves in negative/positive energy region controlled by the applied gate voltage.

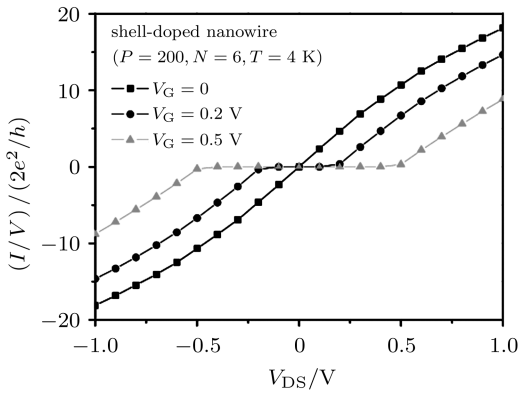


Fig. 2. I–V curves of the perfect nanowires in the presence of gate voltage.

To explore surface disorder effect on conduction performance of the nanowires, in Fig. 3, the I–V curves are plotted with various surface disorder ξ introduced not only by dopant atoms but also surface reconstruction. It can be seen from Fig. 3 that the conductance decreases firstly and then increases with disorder. The heavily doped nanowires approach a metallic regime, which is qualitatively consistent with the experimental values.[18–21] In the presence of surface disorder, the two terminal I–V curves are linear and thus suggest that the electrodes make ohmic contact with the shell-doped nanowires. For $\xi = 2t, 4t, 8t$, the conductance are obtained to be 0.344 $2e^2/h$, 0.088 $2e^2/h$ and 0.15 $2e^2/h$, respectively.

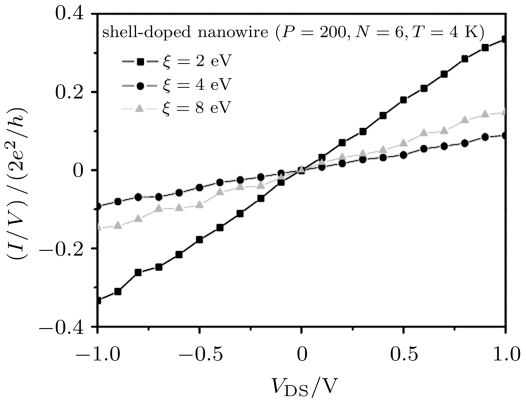


Fig. 3. I–V curves of the shell-doped nanowires at a temperature $T = 4$ K.

To further explore the effect of surface disorder on electron transport, the curve of current as a function of disorder strength is plotted in Fig. 4. It can be seen from Fig. 4 that the current of the shell-doped nanowires exhibits a rather counterintuitive behaviour. In the case of stronger regime ($\xi > \xi_{\rm c}$), the current of shell-doped nanowires increases with increasing ξ, while it decreases in the case of weaker regime ($\xi < \xi_{\rm c}$).

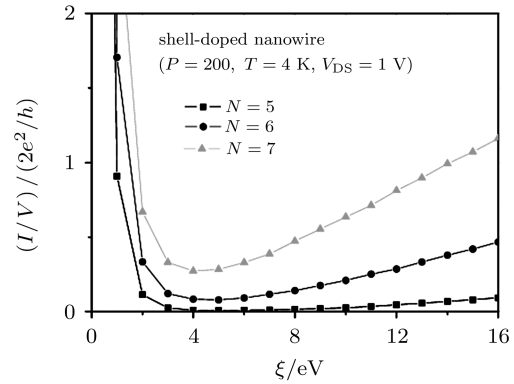


Fig. 4. The average current of the shell-doped nanowires versus disorder strength ξ.

From a more careful analysis, it is found that in the regime of stronger disorder, the conductance almost increases linearly with surface disorder. To shed light on the intrinsic mechanism of the counterintuitive behaviour, the shell-doped nanowire can be considered as a coupled system comprising two subsystems. H_1 and H_2 represent the sub-Hamiltonians of the disordered shell zone and the perfect core. H_{12} and H_{21} are the coupling Hamiltonians. From the Schrödinger equation, we have

$$\begin{pmatrix} H_1 & H_{12} \\ H_{21} & H_2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \tag{1}$$

where ψ_1 and ψ_2 are the corresponding wave functions. Assume that Eq. (1) can be written

$$(H_1 - \alpha)\,\psi_1 = E\psi_1, \tag{2}$$

$$(H_2 - \beta)\,\psi_2 = E\psi_2. \tag{3}$$

According to Eqs. (1), (2) and (3), we can obtain

$$\alpha = H_{12}\,(H_2 - E)^{-1}\,H_{21}, \tag{4}$$

$$\beta = H_{21}\,(H_1 - E)^{-1}\,H_{12}. \tag{5}$$

From the above equations, we can find that for the disordered shell zone, the larger the disorder, the stronger the localisation of electrons. However, β is inversely proportional to ξ. With increasing disorder, thus, the electrons are extended gradually to the perfect core. Because the effect of disorder upon the disordered shell zone is larger than that of the perfect core, a critical disorder value is obtained. Due to $\beta \to 0$ as $\xi \to \infty$, the enhancement of conductance of the shell-doped nanowires can be attributed to the uncoupling between the disordered shell and the perfect core. Therefore, the conductance of nanowires can be controlled through modulation of the disorder strength. In addition, it can be seen from Fig. 4 that at a given $P = 200$, the average conductance increases with $D(D = Na)$. This is because the number of effective paths increases with increasing D. The numerical results show that the quantum size effect plays an important role in determining the conductance in shell doped nanowires.

To further clarify the quantum size effect on the conduction mechanism of shell-one-dimensional doped nanowires, we calculate the current as a function of length L. It is well known that in an infinite 1D system all states are localised even for weak disorder in the system. The conductance is expected to decrease exponentially with length L. In Fig. 5, the current versus length L is plotted. It can be seen from Fig. 5 that the current depends strongly on the sample length (L) and decreases with increasing L. From a more careful analysis, it is found that the currents decline exponentially with L because of the electrons localisation. In the presence of shell dopants, it can be seen from Fig. 5 that the I–L curves corresponding to disorder strength of $2t$ and $4t$ fit well to the equations $I = 4.69\exp(-L/66.74) + 0.047$ and $I = 2.69\exp(-L/58.23) + 0.02$, respectively. This is because in the phase-coherent limit, the conductance of disordered quasi-one-dimensional sample decreases with its length, $g = g_0\exp(-L/L_0)$. Therefore, the

sample length L is also an important factor in current measurement, which should be considered in the current measurement experiment.

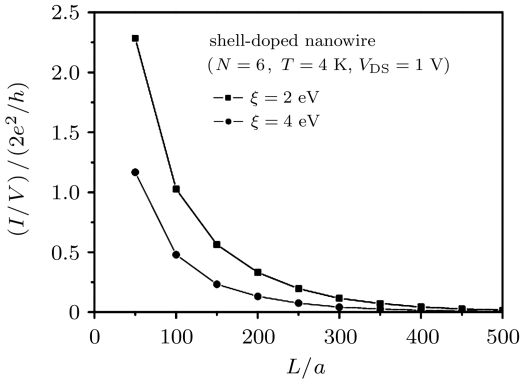


Fig. 5. The current of the shell-doped nanowires as a function of length L.

4. Conclusion

In summary, the conductance and electric currents of the shell-doped nanowires have been calculated. The numerical results show that in the regime of strong disorder, the electric current increases linearly with surface disorder. The heavily shell-doped nanowires approach to a metallic regime. Moreover, the electric current increases with wire diameter (D) and decreases exponentially with wire length (L). These findings may lead to important applications in manipulation of carrier transport not only for shell-doped nanowires of single species but also for coaxial hetero-structured nanowires with modulation of doping.

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