The spin-dependent transport of Co-encapsulated Si nanotubes contacted with Cu electrodes

Yan-Dong Guo,[1,2] Xiao-Hong Yan,[1,2,a)] and Yang Xiao[1]
[1]*College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China*
[2]*College of Electronic Science and Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210046, China*

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Unlike carbon nanotubes, silicon ones are hard to form. However, they could be stabilized by metal-encapsulation. Using first-principles calculations, we investigate the spin-dependent electronic transport of Co-encapsulated Si nanotubes, which are contacted with Cu electrodes. For the finite tubes, as the tube-length increases, the transmission changes from spin-unpolarized to spin-polarized. Further analysis shows that, not only the screening of electrodes on Co's magnetism but also the spin-asymmetric Co-Co interactions are the physical mechanisms. As Cu and Si are the fundamental elements in semiconductor industry, our results may throw light on the development of silicon-based spintronic devices. © *2014 AIP Publishing LLC*.
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Spintronics is one of the most promising areas in nanoelectronics.[1–3] Nowadays, silicon is a fundamental element in semiconductor industry, so it is important to study its application in spintronics. So far, kinds of spin-related phenomena have been revealed in Si-based materials.[4–7] Unlike carbon nanotubes, silicon ones with hollow inside are hard to form, as sp^2 hybridization is not favorable in Si.[8,9] However, it is found that, Si cage clusters could be stabilized by metal encapsulation.[8,10,11] Moreover, they could be assembled together to form Si nanotubes.[12–14] In experiment, epitaxial self-assembled metal silicide nanowires (or nanotube bundles) have been synthesized,[15,16] and their stability as well as other properties have been studied by theoretical studies.[17] Previous studies show that $3d$ transition metal-doped Si nanotubes exhibit interesting magnetic properties,[13,18] which have great potential for fabricating Si-based spintronic devices. In the present work, we focus on the spin-dependent electronic transport of Co-doped Si nanotubes, which are contacted with Cu electrodes. For the finite tubes, as the tube-length increases, the transmission changes from spin-unpolarized to spin-polarized. It is found that, the transition is induced not only by the screening of electrodes on the magnetic moment of Co, but also by the spin-asymmetric Co-Co interactions. As both Cu and Si are the fundamental elements in semiconductor industry, we believe our results are useful for the designing of Si-based spintronic devices.

To explore the transport properties of the system accurately, density functional theory (DFT) calculations combined with nonequilibrium Green's function (NEGF) are performed, which are carried out through the Atomistix Toolkit package.[19,20] We use the mesh cutoff energy of 150 Ry, and $4 \times 4 \times 50$ k-point mesh in the Monkhorst-Park scheme.[21] As the system contains transition metal atoms, Perdew-Burke-Eenzerhof (PBE) formulation of the generalized gradient approximation (GGA) is used as the exchange-correlation function.[22] Double-zeta basis set is chosen to be the local numerical orbitals, with which the transmission spectra are in good agreement with former results.[23] The nanotubes are fully optimized until all the forces are less than 0.05 eV/Å. By minimizing the total energy of the whole system, the distance between electrodes and Si nanotube is optimized to be 2.35 Å.

In NEGF theory, the current is obtained according to the Landauer-Büttiker formula

$$I(V)_{\uparrow\downarrow} = \frac{2e}{h}\int T(E,V)_{\uparrow\downarrow}[f(E-\mu_L) - f(E-\mu_R)]dE,$$

where $\mu_{L/R}$ is the chemical potential of the left or right electrode, $f(E-\mu_{L/R})$ is the Fermi function in the left or right electrode, and $V = (\mu_L - \mu_R)/e$ defines the bias window. $T(E,V)_{\uparrow\downarrow}$ is the transmission probability through the system for up- or down-spin, which is calculated from (the denotation of spin is omitted)

$$T(E,V) = Tr[\Gamma_L(E,V)G^R(E,V)\Gamma_R(E,V)G^A(E,V)],$$

where $G^{R/A}(E,V)$ is the retarded or advanced Green's function of the scattering region, and $\Gamma_{L/R}$ is the coupling matrix to the left or right electrode. In this paper, we focus on the zero-bias ($V = 0$) condition, as the transport under low bias is largely dominated by it.

For clarity, the Co-doped Si nanotubes are denoted as $Si_{6N+6}Co_N$, where N = 1, 2, 3, and 4. The right panel of Fig. 1(b) presents the cross-section of the tubes. Most commonly used materials of electrodes are Cu, Al, Au, and Ag, and they all possess face centered cubic (fcc) structure. Like the cross-section of the Si tube, fcc(111) surface exhibits hexagonal lattice geometry, as shown in Fig. 1(b). Among these four metals, the structural parameter of Cu(111) matches the best with that of Si nanotube [see Fig. 1(b) for details]. Besides, it is a fundamental element in integrated circuit (IC), so Cu is chosen to be the electrode material, with the (111) surface to be the contact surface.

a)Electronic mail: xhyan@nuaa.edu.cn

