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Electronic structure and transport properties of Si nanotubes

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The electronic structure and the transport properties of Si nanotubes with outer diameter between 2 and 20 nm are investigated using fully atomistic simulations. A formula is given for the energy of the band edges versus diameter and thickness. The phonon-limited mobility of electrons and holes is calculated and is compared to the case of Si nanowires. It is found that the thickness of the nanotubes is the main parameter controlling the shape of the band structure and the values of the effective masses. Configurations with expected best carrier mobilities are discussed.

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I. INTRODUCTION

Si nanowires (NWs) with diameters below 20 nm are attractive building blocks for nano-scale and flexible electronics,^{1–3} in particular for ultimate transistors because of reduced short channel effects.^{3–7} However, the coupling of the carriers to impurities, phonons or interface roughness is usually enhanced by the confinement. Hopefully, the electronic bands and the effective masses in NWs are strongly influenced by the quantum confinement and it shall be possible to find a combination of NW diameter (D_{NW}) and orientation with good transport properties, even in some cases better than in bulk Si.^{8–15} Another interesting option is to apply strains on the NWs.^{8,16}

However, the fabrication of ultimate Si NW devices may be quite challenging. In this context, it is highly desirable to explore new ways to play with the quantum confinement in order to tailor the transport properties in a 1D geometry. Si nanotubes (NTs) offer this possibility as we can vary their inner (d_{NT}) and outer (D_{NT}) diameters. In addition, Si NT transistors with core-shell gate stacks should show enhanced performances¹⁷ thanks to a better electrostatic control of the channel. The synthesis of Si NTs has been reported,^{18,19} for example by etching the Ge core of Ge-Si axial NW heterostructures.¹⁹ But the electronic properties of Si NTs are still unknown, motivating the present work.

In this paper, we present a fully atomistic study of Si NTs with D_{NT} between 2 and 20 nm. We show that NTs and NWs have comparable band structure, effective masses, and phonon-limited carrier mobility when they have the same orientation and similar Si thickness ($D_{NT} - d_{NT} \approx D_{NW}$). We conclude that the best transport properties should be achieved in $\langle 001 \rangle$ NTs for electrons, and in $\langle 111 \rangle$ NTs for holes, and that $\langle 110 \rangle$ NTs represent the best compromise for both carriers.

II. METHODOLOGY

The electron band structure of the NTs is computed with the $sp^3d^5s^*$ tight-binding model of Ref. 20, which reproduces

all effective masses and deformation potentials of bulk Si. Spin-orbit coupling is taken into account in the valence bands. We calculate the phonon-limited mobility within a fully atomistic framework.^{12,15,16} For that purpose, we compute the phonon band structures using a Valence Force Field model.²¹ The electron-phonon interactions are obtained from the derivatives of the tight-binding Hamiltonian with respect to the atomic positions. All scattering processes fulfilling energy and momentum conservation are considered. Boltzmann's transport equation is solved exactly for the low-field mobility at low carrier concentration ($T = 300$ K). Details on the methodology are given in Refs. 12 and 15.

III. RESULTS

A. Mobility and effective masses

We first consider a set of NTs with fixed outer diameter $D_{NT} = 10$ nm. In Figs. 1(a) and 1(b), the mobilities of electrons and holes are plotted against the difference $D_{NT} - d_{NT}$. The mobilities in NWs with the same thickness of Si ($D_{NW} = D_{NT} - d_{NT}$) are shown in the same plot. The agreement between the two sets of results is striking, meaning that the thickness of Si NTs plays a role equivalent to the radius of Si NWs, at least for transport properties in this range of sizes. The explanation for this surprising result will be discussed at the end of the paper. Therefore, the trends followed by the mobility versus orientation and thickness are basically the same for NTs and NWs.¹⁵ For electrons, mobility increases with thickness, $\langle 110 \rangle$ NTs perform better for small $D_{NT} - d_{NT} \leq 5$ nm, $\langle 001 \rangle$ NTs otherwise. For holes, $\langle 111 \rangle$ NTs present the best performances, their mobility peaks around $D_{NT} - d_{NT} = 4$ nm and is greater than that of bulk Si in a wide range of thicknesses. However, $\langle 110 \rangle$ NTs represent a good compromise for both types of carriers.

Atomistic calculations of the mobility are limited to $D_{NT} < 10$ nm because they require heavy computational resources. However, as the mobility is inversely proportional to the effective mass m^* , it is interesting to compare the variations of m^* in a wider range of sizes. Therefore, we define the average of the inverse effective mass of electrons as $1/m_e^* = (\sum_i n_i/m_i^*)/n$ where m_i^* and n_i are the effective

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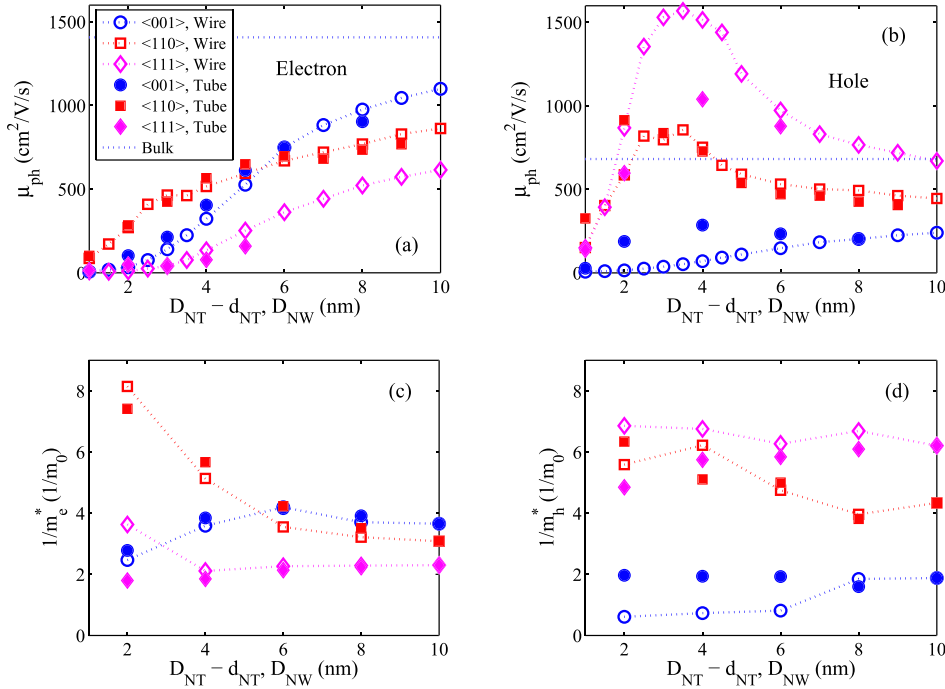


FIG. 1. Electron (a) and hole (b) mobility, electron (c) and hole (d) average inverse effective mass in Si NTs, as function of $D_{NT} - d_{NT}$ with $D_{NT} = 10$ nm, for $\langle 001 \rangle$ (\circ), $\langle 110 \rangle$ (\square) and $\langle 111 \rangle$ (\diamond) orientations. The equivalent data for NWs are shown as function of D_{NW} for comparison. m_0 is the free-electron mass.

mass and the electron density in band i , respectively, and n is the total electron density. A similar formula is used for holes ($1/m_h^*$). In Figs. 1(c) and 1(d), the data for $1/m_e^*$ and $1/m_h^*$ are presented in the same form as the mobilities showed in Figs. 1(a) and 1(b) for direct comparison. It is quite clear that $1/m_{e,h}^*$ and the mobilities have very consistent behaviors for NTs and NWs. The electron effective mass becomes heavier in $\langle 110 \rangle$ NTs than in $\langle 001 \rangle$ NTs when $D_{NT} - d_{NT}$ exceeds 5 nm, and the hole effective mass is always the lightest in $\langle 111 \rangle$ NTs. In addition, NTs and NWs with the same thickness have quite similar effective masses. Of course, the variations of the mobilities are not entirely defined by those of $1/m_{e,h}^*$. For example, m_e^* is the lightest at $D_{NT} - d_{NT} = 2$ nm in $\langle 110 \rangle$ NTs while the mobility is very low; m_h^* is almost constant in $\langle 111 \rangle$ NTs while the mobility has a marked peak. These differences can obviously be attributed to changes in scattering rates. In NTs with small diameter, electron-phonon scattering is significantly enhanced^{13–15} due to the confinement. Also, inter-subband scattering is enhanced when bands become closer, and it is the reason why the hole mobility decreases as NTs get thicker.¹⁵ However, Fig. 1 demonstrates that a light effective mass is a key factor to achieve high mobility.²²

On this basis, we consider NTs with fixed thickness ($D_{NT} - d_{NT} = 4$ nm). Figure 2 shows that $1/m_{e,h}^*$ does not vary much when d_{NT} changes from 4 nm to 16 nm. Also, the effective masses are very light for both electrons and holes in the best orientations. This shows that thickness is the predominant factor controlling the average effective mass in NTs (at least for this range of size), and that NTs with large diameter are likely to achieve the highest electron (hole) mobility for $\langle 110 \rangle$ ($\langle 111 \rangle$) orientation. Interestingly, light effective masses are predicted for both electrons and holes in $\langle 110 \rangle$ NTs.

The mobilities shown in Fig. 1 have been computed at low carrier density, where the current is mostly limited by

electron-phonon interactions.^{23,24} At larger carrier density, for example, above $\approx 4 \times 10^6$ cm⁻³ in Si NWs with $D_{NW} = 8$ nm,²⁴ surface roughness scattering comes into play

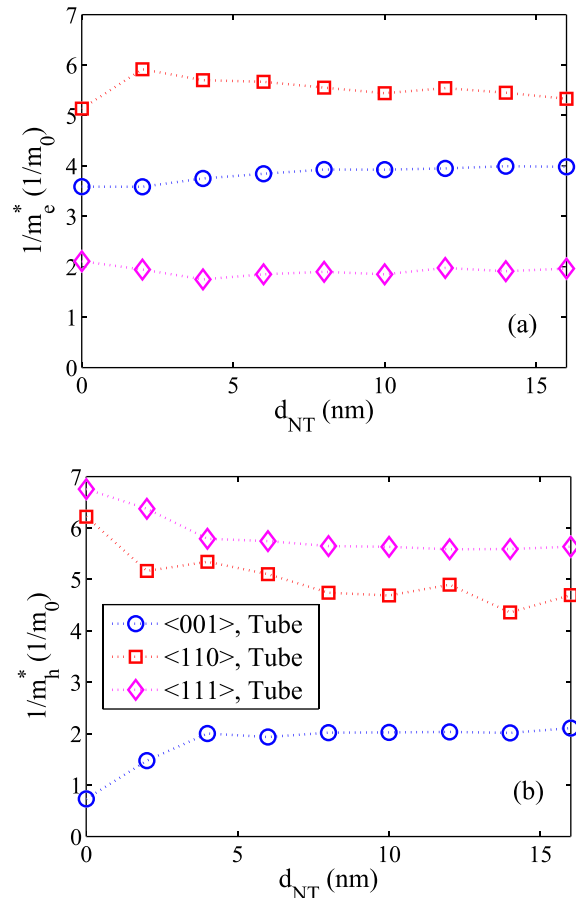


FIG. 2. Electron (a) and hole (b) average inverse effective mass as function of the inner diameter d_{NT} in NTs with $D_{NT} - d_{NT} = 4$ nm, for $\langle 001 \rangle$ (\circ), $\langle 110 \rangle$ (\square) and $\langle 111 \rangle$ (\diamond) orientations. m_0 is the free-electron mass.

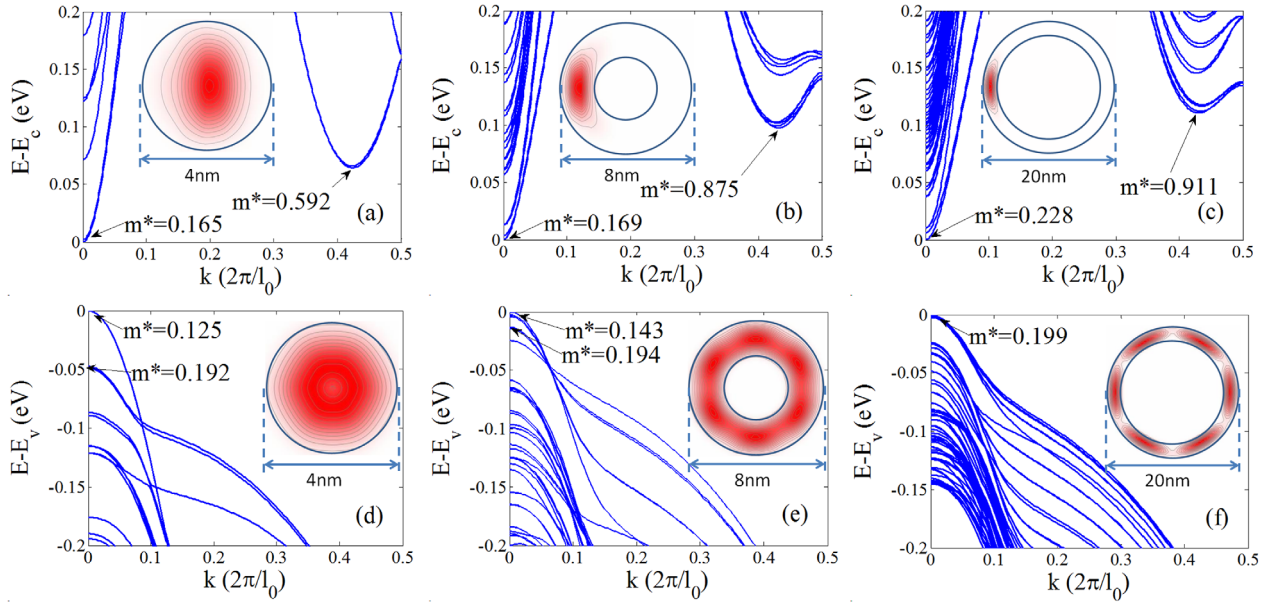


FIG. 3. Electron (a–c) and hole (d–e) band structures for $d_{\text{NT}} = 0$ (a,d), 4 (b,e), 16 nm (c,f), for NTs with fixed thickness $D_{\text{NT}} - d_{\text{NT}} = 4$ nm. The NTs have $\langle 110 \rangle$ (a–c) or $\langle 111 \rangle$ (d–e) orientation. l_0 is the length of the unit cell; E_c and E_v are the conduction and valence band edges, respectively. The insets show density plots of the wave functions at the band edges. The localization of the wave functions at one side of the NTs (b,c) is induced by very small asymmetry in the structures.

and the mobility is further degraded. The influence of surface roughness is certainly worse in NTs, since two surfaces are present. But simulations of these effects require Non-Equilibrium Green's Function (NEGF) calculations, which cannot be performed in tight-binding for the NT sizes investigated here. In principle, NEGF calculations based on a $\mathbf{k} \cdot \mathbf{p}$ model are feasible^{23,24} but are beyond the scope of the present work. However, even when surface roughness scattering becomes predominant, we expect that the ordering of the mobility versus NT orientation will be the same as for the phonon-limited mobility, as already shown for NWs.²⁴ In other words, NT orientations giving the smallest effective

masses should present the best transport properties even at high carrier density.

B. Band structures

The analysis of the band structures and wave functions of NTs give better insight into these results. We find that NTs of the same thickness actually have band structures with similar shape. For illustration purposes, we selected three NTs (NWs for $d_{\text{NT}} = 0$) with the best orientation for each carrier. Figures 3(a)–3(c) show that the conduction band edge of $\langle 110 \rangle$ NTs is at $k = 0$ with light effective mass

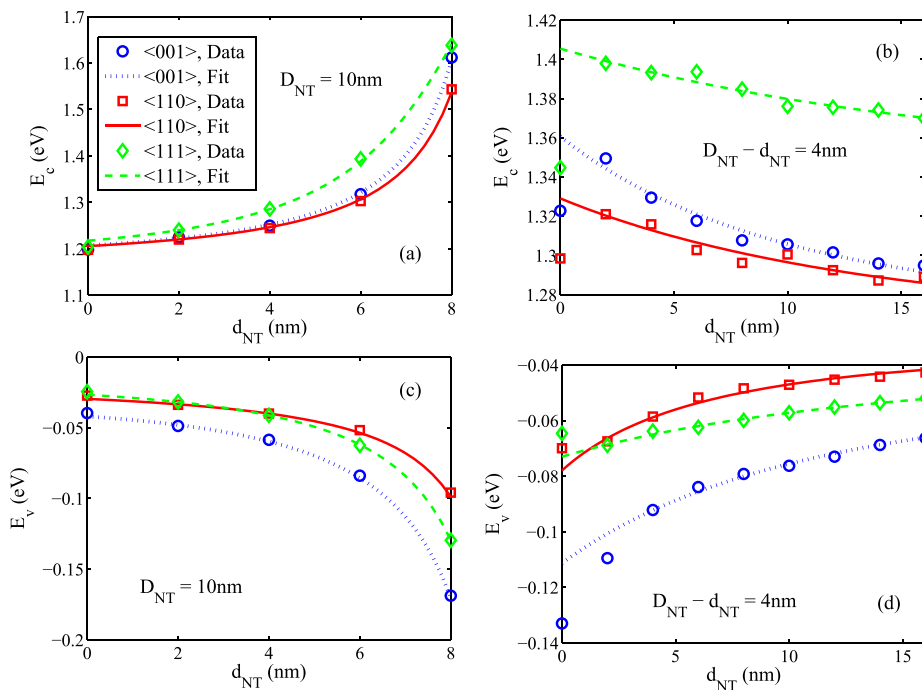


FIG. 4. Conduction and valence band edges as function of the inner diameter d_{NT} of NTs with fixed outer diameter $D_{\text{NT}} = 10$ nm (a,c) or with fixed thickness $D_{\text{NT}} - d_{\text{NT}} = 4$ nm (b,d), for $\langle 001 \rangle$ (\circ), $\langle 110 \rangle$ (\square) and $\langle 111 \rangle$ (\diamond) orientations.

TABLE I. Parameters of Eq. (1) fitting band edge energies of Si NTs. The values are given for energies defined in eV and diameters in nm.

Edge	E_∞	Orientation	K	C_1	C_2	C_3	C_4	C_5
E_c	1.172	$\langle 001 \rangle$	4.18	0.73	-1.75	2.05	-1.95	-2.04
		$\langle 110 \rangle$	4.65	0.71	-1.72	3.30	-3.52	0.23
		$\langle 111 \rangle$	4.34	0.97	-1.98	-0.49	0.67	4.74
E_v	0	$\langle 001 \rangle$	17.99	2.20	-3.09	-50.36	46.87	32.83
		$\langle 110 \rangle$	-1.72	0.09	-1.14	1.92	-2.08	3.90
		$\langle 111 \rangle$	-1.56	0.77	-1.79	2.86	-2.62	-0.82

($\approx 0.2m_0$). The electron band with heavier effective mass is at about $k = 0.4$ and higher in energy so that it does not affect $1/m_e^*$ much. Figures 3(d)–3(f) show that the effective mass of the first valence band in $\langle 111 \rangle$ NTs is quite small, while the effective mass of the next few valence bands is slightly heavier. Although the first few bands come closer with increasing diameter, their effective masses remain small. For both conduction and valence bands, NTs with larger diameter show more bands near the edge, but there is still a small gap between the first and the second group of bands which must reduce inter-subband scattering.

Figures 3(a)–3(c) also show that the electron wave functions at the band edges in NTs and NWs do not have a cylindrical symmetry. In NTs, they even present localized lobes across the section. This results from the strong anisotropy of the band structure and effective masses in bulk Si. Interestingly, the electron wave functions of Figs. 3(a)–3(c) present a similar degree of localization when compared on the same scale (not shown). This qualitatively explains why the mobility is surprisingly controlled by the total thickness, and not by the cross section area for example, at least in this range of size. In the case of holes, the wave functions are more symmetric, especially in the $\langle 111 \rangle$ orientation [Figs. 3(d)–3(f)], as the hole confinement masses are heavier and less anisotropic. It is also in that case that the mobility in NTs and NWs with the same thickness presents the largest discrepancy (Fig. 1).

C. Confinement energies

Finally, we discuss the effect of quantum confinement on the energy of the band edges. Figures 4(a) and 4(c) illustrate the effect of thickness when we vary d_{NT} ($D_{\text{NT}} = 10$ nm). Figures 4(b) and 4(d) show the effect of the diameter when thickness is fixed. The monotonicity of band edges as function of d_{NT} breaks at $d_{\text{NT}} = 0$ nm, which stands for NWs. This is expected as the boundary condition for NTs and NWs is different. The energy of NT band edges can be reproduced by the following formula:

$$E = E_\infty + \frac{K}{D^2 + C_1 d^2 + C_2 Dd + C_3 D + C_4 d + C_5}, \quad (1)$$

where E_∞ is the bulk value ($d \equiv d_{\text{NT}}, D \equiv D_{\text{NT}}$). The parameters C_{1-5} and K (Table I) were obtained by fitting 28 band edges of NTs. Equation (1) is only valid for

$2 \leq d_{\text{NT}} < D_{\text{NT}} \leq 20$ nm. For NWs, the expressions are given in Ref. 25.

IV. CONCLUSION

In conclusion, we have investigated the electronic structure and the transport properties of Si NTs in a wide range of diameters. We have compared NTs with NWs of the same thickness, and we have found that they present band structures with quite similar shape and close values of electron (hole) average effective mass. These findings indicate that the thickness of NTs is a pertinent parameter controlling the transport properties. Si NTs with light effective masses can be found for certain orientations, strengthening their potential interest for performant nanoscale transistors.¹⁷

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