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PREDICTION OF ELECTRON DRIFT VELOCITY IN HELICALLY COILED CARBON NANOTUBES

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Abstract: We studied electron transport in single wall carbon nanotubes placed in stationary homogeneous electric fields, oriented along tubes. Electron distributions for various electric fields are determined by solving stationary multi bands Boltzmann transport equation in presence of electron phonon scattering mechanisms. Contributions of all possible scattering channels, allowed by selection rules and energy conservation, are taken into account for finding scattering rate and collision integrals. As it is previously predicted, large electron drift velocities in straight single wall carbon nanotubes are obtained. Frequent electron scattering as well as low group velocity have strong impact on reduction of drift velocity in helically coiled carbon nanotubes.

Keywords: helically coiled carbon nanotubes, electron-phonon interaction, drift velocity.

1. INTRODUCTION AND MODEL OF HCCNT

High electron mobility in a weak electric field certainly belongs among very important physical properties of carbon nanotubes. For straight single wall carbon nanotubes (SWCNTs) this phenomena is theoretically detaily explained and shortly afterward experimentally confirmed [1]. These predictions are important for application of nanotubes as interconnects or transistors. Unique physical properties of carbon nanotubes (CNTs) among which are high elasticity and various electrical performances, makes them candidate for construction of nanoelectromechanical short devices. Ultrahigh mass sensitivity in combination with low mass density and high electron mobility of CNTs still attract attention of many researches. While except predictions of mechanical properties related with extreme elasticity a little is known about current caring performances of helically coiled carbon nanotubes (HCCNTs).

In this paper are given predictions for charge transport properties of a straight and a helically coiled carbon nanotubes. In order to find electron mobility dependence on electric fields, oriented along tube axis of SWCNTs or along helix axis for HCCNTs, we used solutions of stationary Boltzmann transport equations. Collision operator in transport equation is modeled such that contain only meaningful scattering mechanisms, electron-phonon scattering. Essential for determining strength of electron-phonon (el-ph) interaction in tight binding picture is knowledge of electron and phonon spectra. In calculations both models of CNTs are considered as perfect crystal lattice, without effects of impurities or defects. Here we focused on carrier transport properties of semiconducting carbon nanotubes, assuming that they are doped, such that Fermi level crosses lowest unoccupied state of conducting band.

Transport characteristics are determined for realistic model of helically coiled carbon nanotubes. Monomer of used model of HCCNTs, except hexagons, includes pairs of pentagons and heptagons. Five and seven carbon rings are placed on positive and negative Gaussian curvature respectively, providing stability of helical structure. Whole model of HCCNT is generated from set of atoms called symmcell, applying line group from the fifth family. Primarily monomer is built from symmcell acting with rotation around x axis for π. Afterwards rest of the model is generated by action of the screw axis elements: rotation followed by fractional translation. Arrangement of the monomer of HCCNT with pentagons, hexagons and heptagons is written with (n_6, nr, n_7, n_5, ($\boldsymbol{b}_1$, $\boldsymbol{b}_2$)) and have been detailed explaned in [2,3]. First four numbers in label of helical nanotube model (n_6, n_r, n_7, n_5) are parameters of the graph plane, which is

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fundamental for construction of model and define numbers of atoms in monomer as well as contribution of specific polygons. Supercell vectors ($\boldsymbol{b}_1$, $\boldsymbol{b}_2$) determined orientation of particular polygons into the monomer. Mathematical theory well known as topological coordinate method, which is based on graph theory, is used to construct the presented HCCNT model. We upgraded initially proposed model from [4] through development of new graphs, which is used for modeling various atomic structure and further generating HCCNTs with realistic geometrical parameters.

2. ELECTRON-PHONON INTERACTION AND BOLTZMANN TRANSPORT EQUATION

When external electric field is applied current flow occurs along CNTs, such that electrons accelerate until they crossing into another states over absorbing or emitting of phonon, and these processes are repeated. Here, we consider scattering rate (W), originated only from electron-phonon interaction, while all other scattering mechanisms are neglected. Scattering events happen instantaneously, much shorter than electron free flight time. Instead of steady-state Fermi-Dirac distribution function, when electric field is applied electrons are distributed with nonequilibrium distribution function. Population of an electron state $f(k,m)$ from conducting band, with angular quantum number m and wavevector k, depends on electric field and scattering rate [5]. This electron momentum distribution satisfies Boltzmann transport equation given as

$$\frac{e}{\hbar}E\nabla f(k,m) = -\sum_{k',m'}\left[W(k',m';k,m)f(k',m')\left(1-f(k,m)\right) - W(k,m;k',m')f(k,m)\left(1-f(k',m')\right)\right].$$

which is solved numerically [6] with commonly used simplification, known as low density approximation $f(k,m) \ll 1$. All permitted channels [15] are found numerically and accounted in total scattering rate of accelerated electrons, often distributed in different bands. In order to calculate electron drift velocity (v_d) total momentum distribution function is required over all relevant conducted bands Fig. 1. Transition probability from initial (k,m) into the final electron state (k',m') over emitting or absorbing phonon per unit time is estimated from Fermi's golden rule, expressed with

$$W\left(k',m';k,m\right) = \frac{2\pi}{\hbar}\left|\mathcal{M}_{\pm}^{\nu q}\left(k',m';k,m\right)\right|^2 \delta\left(\varepsilon_m(k) - \varepsilon_{m'}\left(k'\right) \pm \hbar\omega_\nu(q)\right).$$

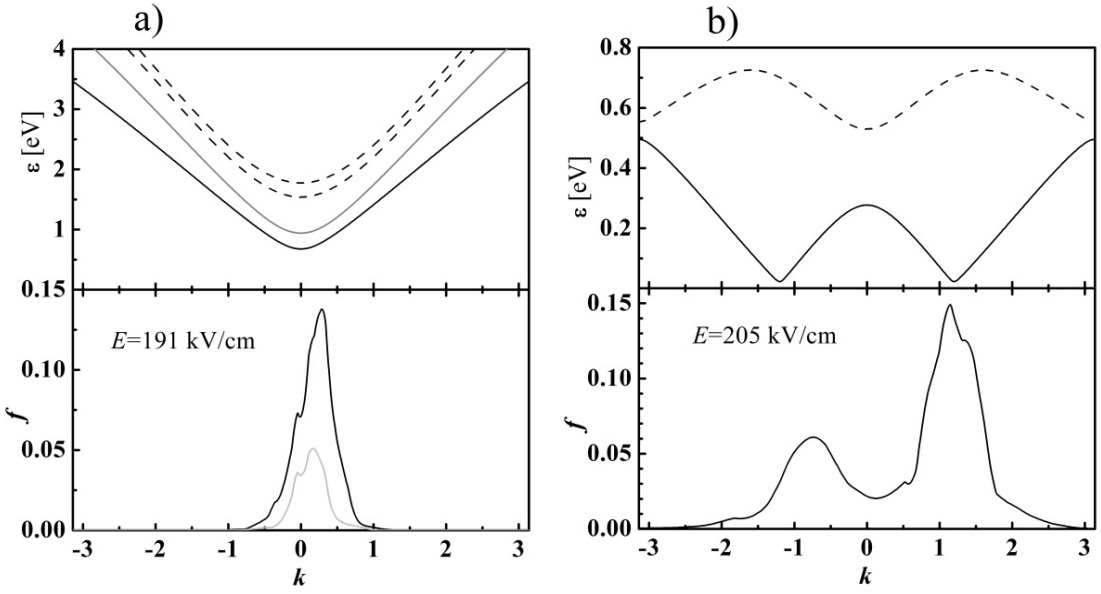

Figure 1. Conducted bands (upper panel), plotted with solid lines have significant distribution function (lower panel) at 300 K, while otherwise they are plotted with dashed lines for (11,0) SWCNT in a) and (2,3,4,0,((1,0),(0,5))) HCCNT in b).

Electron transition through emission (+) or absorption (-) of phonon has nontrivial probability if selection rules and energy conservation are satisfied. Each conducted state in HCCNTs has many

scattering channels with significant contributions to the total scattering rate. All types of processes in and outside of the first Brillouin zone, named as *normal* and *umklapp* processes respectively, with fulfilled selection rules for angular quantum number and wavevectors are efficiently selected by applying theory of group projector thoroughly explained in [8,9]. When the triples of states that constitute scattering channels are determined, than the main obstacle in further calculation of *W* is determining of electron-phonon matrix elements $\mathcal{M}_{\pm}^{\nu q}\left(k^{'},m^{'};k,m\right)$ [15], described as coupling between initial and final electron states with the phonon (q,ν). In order to predict charge transport properties, mostly are required phonons from the middle of Brillouin zones, which produce nonhomogeneous lattice deformation. While approximation of deformation potential obtained only using Γ point phonons is insufficient to describe all relevant transitions.

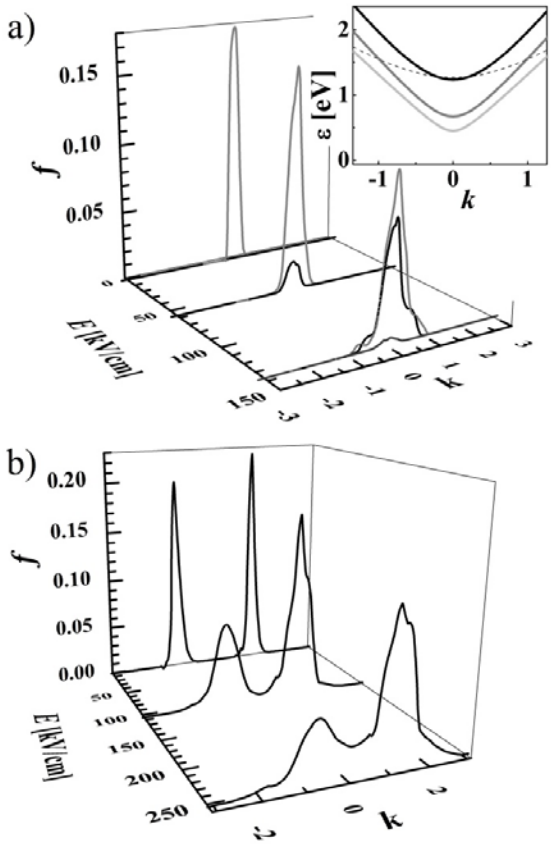

Figure 2. a) Conducting bands and appropriate electron distribution for (17,0) SWCNT given at different E have the same color. b) Distribution function in conducted band of (2,3,4,0,((1,0),(0,5))) HCCNT at various electric field. Distribution functions at 300 K are presented.

Determination of electron-phonon matrix elements is done in extended tight binding scheme, using atomic deformation potentials for sp^3 hybridization. Values of atomic deformation potential are obtained from density functional theory [11], and their using is completely described in [7].

Intensity of el-ph coupling depends on coefficients of initial and final electron wavefunctions, as well as vector polarization of phonon involved in the given process. Movement amplitude or occupancy of phonon states are function of temperature and determined by Bose-Einstain distribution function. Electron and phonon spectra, used for calculation of el-ph matrix elements, are obtained with a help of modified group projector, whose theory is in detail explained in [8,10]. Using Brenner semiempirical interatomic potential for carbon atoms in solids [12,13] each helically coiled carbon nanotube is relaxed, and further for each one of them are calculated harmonic force constants, necessary for construction of phonon Hamiltonian. Due to the lack of rotational symmetry all phonon and electron dispersion branches have angular quantum number 0. As a consequence of trivial angular quantum number selection rules in HCCNTs are only restrictions for wavevectors, and certainly energy conservation must be fulfilled.

Obtained distribution function depends on strength of applied electric field (*E*) Fig. 2 as well as temperature through intensity of scattering rate. Deviation of distribution function from the equilibrium one is larger when NT is in stronger field, while peak of *f* is shifted to the states with higher energies. When conducted band has two local minima like in (2, 3, 4, 0, ((1, 0), (0, 5))) HCCNT Fig 1 b), nonequilibrium distribution function has two asymmetric peaks at finite electric field. In vicinity of Van Hove singularities scattering rate rapidly increases, affects fast changes of distribution function in vicinity of high density states. Electron occupation of high density states in upper conducted band of zig-zag SWCNTs becomes significantly through interband transition induced by increasing of electric field.

3. RESULTS

In helically coiled and straight NTs peaks of nonequilibrium electron distribution function shifts to the electron states with larger group velocities when intensity of electric field gradually changes from *E*=0. Intraband transitions occur for all values of *E* and affect spreading of distribution around Fermi level. From appropriate intensity of applied filed in zig-zag semiconducting SWCNTs interband transitions occur and becomes more frequent with further increasing of *E*. Filling of the states in the

upper conducted bands induced with applied electric field begins in vicinity of Γpoint (k=0) Fig. 2 a). Frequently interband transitions in zig-zag SWCNTs result in drop of the drift velocity due to the filling of the states with lower group velocity. Further increasing of electric field leads to the negative differential mobility [15].

Conducting electrons in (2, 3, 4, 0, ((1, 0), (0, 5))) HCCNT are distributed in the states around local minima, symmetrically in correspondence to the k=0 in the absence of an electric field. When field increases electrons become more localized in vicinity of the one local minimum Fig. 2 b). Even then, occupation of upper conducting band of the given HCCNT is negligible. Despite that, negative differential mobility appears in HCCNT Fig. 3, via increasing electron occupation in the states around Γ point Fig. 1 b). Related to the lack of the rotational symmetry of HCCNTs, all their electron and phonon bands have angular quantum number 0. In accordance with non-crossing rule, there is not intersection of the bands and they are densely packed into the standard energy ranges. As a consequence, electron zones of HCCNTs are placed in short energy interval and generally their group velocity is downshift in comparison with bands in SWCNTs.

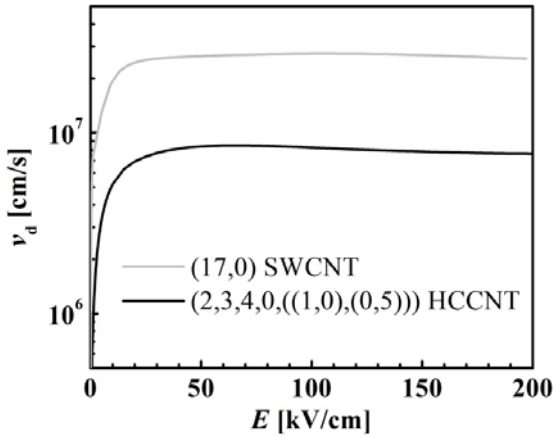

Figure 3. Drift velocity dependence on electric field intensity for semiconducting CNTs at 300 K.

Reduced selection rules is related with increased number of scattering channels, and together with densely packed electron end phonon bands of HCCNTs makes that width of electron distribution function is very sensitive to the variation of electric field intensity. Occupation of states with low group velocity becomes significant at high electric field due to the spreading of *f*, besides maximal group velocity is in short range of wavevectors from Brillouin zone, and all together affects that peak of drift velocity of HCCNTs is remarkably reduced than in SWCNTs as it is shown in Fig. 3. Obtained numerical results of electron drift velocity in applied electric field for zig-zag nanotubes are in agreement with previously predicted and measured values [14,16]. Taking into account scattering rate and band structure of HCCNTs, given estimation of their v_d dependence on electric field is expected. For the given HCCNTs critical electric field, when v_d reaches to maximum, is shifted to the lower intensity of E Fig 3. This indicates that distribution function becomes more delocalized even at low applied field, such that states with low group velocity are significantly occupied.

4. CONCLUSION

Scattering rates for all conducted state in carbon nanotubes are found applying perturbation method, accounting contribution of all allowed scattering channels, determined from electron and phonon dispersion branches using selection rules and energy conservation law. Electron and phonon bands as well as electron-phonon matrix elements of HCCNTs and SWCNTs models are efficiently calculated with the help of symmetry based approach. Momentum distributions function at various electric fields as a solution of Boltzmann transport equation is found, and then appropriate drift velocity. Peaks of electric field dependence of drift velocity for HCCNTs are several times lower than in SWCNTs and shifted to the lower values of electric field. Negative differential mobility in HCCNTs is mostly affected over intraband transitions into the states with low group velocities.

5. ACKNOWLADGEMENT

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ЕЛЕКТРОНСКА МОБИЛНОСТ КОД ХЕЛИКАЛНИХ УГЉЕНИЧНИХ НАНОТУБА

Сажетак: Захваљујући слабом спрезању електрона са акустичким фононима угљеничне нанотубе поседују велику електронску мобилност. Проучавали смо електронске брзине дрифта хеликалних и правих једнослојних угљеничних нанотуба у хомогеногеном електричном пољу оријентисаном дуж осе хеликса односно главне осе тубе.

Укупна учесталост расејања добијена је сумирањем свих независних доприноса електрон-фонон расејања, одређених селекционим правилима и законом одржања енергије. Електронска дистрибуција рачуната је за различите интензитете електричног поља, добијена је нумерички решавањем вишезонских Болцманових транспортних једначина, решаваних у инверзном простору. Код хеликалних нанотуба нађене су атипичне вредности и положаји максимума зависности брзине дрифта од интензитета електричног поља.

Кључне речи: хеликалне угљеничне нанотубе, електрон-фонон интеракција, електронска мобилност.