Strong Enhancement of High Voltage Electronic Transport in Chiral Electrical Nanotube Superlattices

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We consider metallic carbon nanotubes with an overlying unidirectional electrical chiral (wavevector out of the radial direction, where the axial direction is included) superlattice potential. We show that for superlattices with a wavevector close to the axial direction, the electron velocity assumes the same value as for nanotubes without superlattice. Due to an increased number of phonons with different momenta but lower electron-phonon scattering probabilities, we obtain a large enhancement of the high-voltage conductance and current sustainability in comparison with the nanotube without superlattice.

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Depending on their chirality, carbon nanotubes (NT) behave either like a semi-conductor or a metal. In the first case, they offer interesting alternative for building logical circuits. In the second case, they can be used as nanometer-sized metallic wires in logical circuits. This is particularly useful since they can sustain very high currents before breaking. At low voltages ($U \lesssim 0.17\text{V}$) the effective electron scattering length at room temperature in metallic NTs is mainly governed by acoustical phonon and impurity scattering with a value of a few hundred nanometers [1]. At higher voltages, scattering with hot optical phonons created by electron-phonon scattering becomes relevant. This leads to a significant reduction of the electron’s mean free path down to roughly $l_{sc} \approx 10\text{ nm}$ [2,3], resulting in a large increase in the absolute and differential resistance. Due to the large number of optical phonons, phonon-phonon scattering with acoustic phonons produces heat in the NT that ultimately causes the electrical breakdown [2,3].

In Ref [5] it was argued that the performance of a metallic NT, i.e., its absolute and differential conductance, can be enhanced considerably by isotropical disorder enrichment. This causes additional relaxation paths for optical phonons by disorder scattering. The purpose of the present letter is to propose a different mechanism to enhance the electronic transport. We show that by applying an unidirectional electrical superlattice (SL) (cf. Fig. 1) with wavevector close to the axial direction of the NT, we can enhance the (differential) conductance considerably, especially in the large voltage regime. Such a potential could be for example produced by adatom deposition via electron beams directed on the NT [10] or (at least approximately) by twisted periodical patterned top and bottom gate electrodes or the coupling of the NT to surface acoustic waves [11]. Since the (average) phonon number is proportional to the inverse electron-phonon scattering time $1/\tau_{ep}$, and the inverse electron mean-free path $1/l_{sc}$ is proportional to the phonon number times $1/\tau_{ep}$ in the hot phonon regime, we obtain a quadratic dependence of the electron mean-free path on the scattering time $l_{sc} \sim \tau_{ep}^{2}$. Below it will be shown that an application of an electrical chiral potential causes a large number of different phonons to take part in the electron-phonon scattering process with increased electron-phonon scattering times, so that $1/\tau_{ep} \sim \sum_{\ell} 1/\tau_{ep}^{\ell}$. This is what causes the strong decrease of the (differential) resistance that scales with $1/l_{sc} \sim \sum_{\ell} 1/\tau_{ep}^{2} \ll 1/\tau_{ep}^{2}$ by using Matthiessen’s rule and reduces the phonon temperature.

It was shown recently that new Dirac points in the energy spectrum can be opened by imposing an SL on the graphene lattice [12–16]. This is also seen in NTs for potentials with wavevector in the radial direction. We will show that they vanish for general chiral potentials.

The Hamiltonian near the Dirac point $K$ for a NT with axis in $y'$ direction subjected to an SL potential reads

$$H_{K} = \left(\begin{array}{ccc} V(x' + t_{\gamma} y') & -i\hbar v_{F}(\partial_{x'} - i\partial_{y'}) & 0 \\ -i\hbar v_{F}(\partial_{x'} + i\partial_{y'}) & V(x' + t_{\gamma} y') & 0 \\ 0 & 0 & 0 \end{array}\right) ,$$

where $v_{F}$ is the Fermi velocity. For a NT with circumference $D$, the SL potential $V$ is periodic in the radial (axial) direction with periodicity $d/d(\gamma t_{\gamma})$, i.e., $V(x' + d) = V(x')$ and one has $D/d \in \mathbb{N}$. In the following we solve the eigenvalue equation $H_{K}\Psi(r') = c\Psi(r')$. We use the abbreviation $t_{\gamma} = \tan(\gamma)$ where $\gamma$ is the chiral angle of the SL potential. The metallic NT boundary conditions are given by $\Psi(x' + D, y') = \Psi(x', y')$.\textsuperscript{17}

To solve the eigenvalue equation we follow first a transfer matrix method similar to Ref. \textsuperscript{14} By using the coordinates $x = x' + t_{\gamma} y'$ and $y = y'$, the solution of the Schrödinger equation has the Bloch form $\Psi(r') = e^{iqy}(u_{1}(x), u_{2}(x))^{T}$ with $(u_{1}(x), u_{2}(x))^{T} = \Lambda(x)(u_{1}(0), u_{2}(0))^{T}$, where

$$\Lambda(x) = e^{-i\hat{q}x}\mathcal{P}\exp\left[\int_{0}^{x} dx' M_{V}(x')\right] ,$$

$$M_{V}(x) = \left(\begin{array}{ccc} q/T_{\gamma}^{2} & i\kappa(x)/(1 + it_{\gamma}) & 0 \\ i\kappa(x)/(1 - it_{\gamma}) & -q/T_{\gamma}^{2} & 0 \\ 0 & 0 & 0 \end{array}\right)$$

and $\hat{q} = qt_{\gamma}/T_{\gamma}^{2}$, $\kappa(x) = [e - V(x)]/\hbar v_{F}$, $T_{\gamma} = \sqrt{1 + t_{\gamma}^{2}}$. The operator $\mathcal{P}$ indicates path ordering and places all
larger values of \( x \) to the left. The Bloch condition reads \((u_1(d), u_2(d))^T = e^{i\eta}(u_1(0), u_2(0))^T \) with \( \det[e^{i\eta} - \Lambda(d)] = 0 \) when \( d \) is the SL wavelength.

Consider first a carbon NT in a chiral periodical lattice of two piecewise constant potentials of the form

\[
V(x) = \begin{cases} 
V_1 & \text{if } 0 \leq x < d_1 \\
V_2 & \text{if } d_1 \leq x < d_1 + d_2.
\end{cases}
\]

Then we obtain \( \Lambda(d) = \Lambda_1 \Lambda_2 \), where \( d = d_1 + d_2 \).

\[
\Lambda_i = e^{-i\eta d_i} \left\{ \cos[\alpha_i(d_i)] + \sin[\alpha_i(d_i)] M V_i d_i \right\},
\]

\[
\alpha_i(d_i) = d_i \sqrt{\kappa^2_i / T^2_\gamma - q^2 / T^2_\gamma}.
\]

\( \kappa_i \) is given by \( \kappa(x) \), with \( V(x) = V_i \). Since \( \det[e^{i\eta \kappa} \Lambda(x)] = 1 \) we have for the eigenvalues of the matrix \( \Lambda(d) \), \( \xi = e^{-i\eta d/(1/2)(T \pm \sqrt{T^2 - 4}) \), with \( T = \text{Tr}[e^{i\eta \kappa} \Lambda(d)] \) and

\[
T = 2 \cos[\alpha(d_1)] \cos[\alpha(d_2)]
\]

\[
+ 2 \sin[\alpha(d_1)] \sin[\alpha(d_2)] \left( \frac{q^2}{T^2_\gamma} - \frac{\kappa_1 \kappa_2}{T^2_\gamma} \right) d_1 d_2.
\]

By taking into account that \( T \) is real, we obtain from \( \textbf{7} \) the dispersion relation

\[
2 \cos(\tilde{q} d + \eta) = T.
\]

In the following, we restrict ourselves to mirror symmetric potentials \( V_1 = -V_2 = V \), with \( d_1 = d_2 = d/2 \) leading to the best current-voltage results over all two-step potentials. This leads to an energy spectrum that possesses a mirror symmetry at \( \epsilon = 0 \) for \( q \) values of the quasi-momentum \( q \) in \( y \)-direction. For \( \epsilon = 0 \), we obtain from Eq. \( \textbf{8} \) that \( T = 2 + q^2 d^2 \sin^2[\alpha_0(d/2)]/\alpha_0^2(d/2)T^2_\gamma \). This leads with \( \textbf{8} \) to the existence of new Dirac points \( \textbf{14} \) at zero chirality \( \tau_{\gamma} = 0 \). The number of these points is given by \([V d/2\pi \hbar v_F T_\gamma]\) where \( |x| \) is the largest integer number smaller than \( x \). For \( \tau_{\gamma} \neq 0 \) an energy gap is opened and the Dirac points disappear (see left panel in Fig. \( \textbf{1} \)).

Next we calculate the energy values of the bands at zero momentum \( q = 0 \). Eqs. \( \textbf{7} \) and \( \textbf{8} \) delivers for these energy values \( \epsilon^0(0) = (\pm \eta + 2\pi n)T_\gamma \hbar v_F / d \) where \( n \) determines the energy bands for fixed quasi-momentum \( \eta \). Thus the energy bands are far more separated in energy space for \( \tau_{\gamma} \gg 1 \) than for the system without chiral potential, i.e. \( \epsilon^0(0) \) for \( \tau_{\gamma} = 0 \).

In order to see how the lowest energy band scales with \( V \) and \( \tau_{\gamma} \), we calculate from \( \textbf{7} \) the energy dispersion of the lowest band for metallic NTs, i.e. \( \eta = 0 \), in the regime \( |\epsilon_s| \ll \hbar v_F T_\gamma / d \), \( V \) and \( q^2 \ll T^2_\gamma (V(x) / \hbar v_F)^2 \), to be called \( \mathcal{R} \). We then obtain

\[
\epsilon_s = \hbar v_F \sqrt{\frac{|\Gamma|^2}{T^2_\gamma} + 4 T^2_\gamma d^2 \sin^2\left(\frac{\tilde{q} d}{2}\right)},
\]

\[
\Gamma = \frac{1}{d} \int_0^d dx \exp \left[ i 2 \int_0^x dx' \text{sgn}[V(x')]\alpha_0(x')/x' \right]
\]

where \( s = \pm 1 \) and \( \text{sgn}[x] \) is the sign of \( x \). Note that \( \Gamma = \sin[\alpha_0(d/2)] e^{i\alpha_0(d/2)/\alpha_0(d/2)} \) for the symmetric two-step potential \( \textbf{3} \).

In Fig. \( \textbf{1} \), we plot the two lowest energy bands \( (d = D) \) for \( \eta = 0 \), by solving Eq. \( \textbf{8} \) numerically. Eq. \( \textbf{4} \) leads to the electron velocity \( v_F(q) = \partial \epsilon_s / \partial (\hbar q) \) along the NT axis (the \( q \) dependency of \( \tilde{q} \) has to be considered in the derivate). We restrict our discussion to momentum region near the Dirac point, i.e., \( \tilde{q} d/2 \ll 1 \). It is smaller for larger potentials \( V \) being maximal at \( \alpha_0 \rightarrow 0 \) with value \( v_F(q) \leq v_F \). We point out that in general for \( |\tau_{\gamma}| \geq 1 \) we have \( v_F(q) \approx v_F \) in \( \mathcal{R} \) irrespective of the potential strength \( V \). Since electron-phonon scattering times are proportional to \( v_F(q) \) we restrict our transport calculations below to NTs with \( |\tau_{\gamma}| \geq 1 \) leading to the largest conductivities. For the group velocity of the electrons in radial direction we have \( v_{Fr}(q) = \partial \epsilon_s / \partial (\hbar q) - t_\gamma v_F(q) \). For \( \tau_{\gamma} \geq 1 \) we obtain \( v_{Fr}(q) \approx v_F(1 - |\Gamma|^2)/T_\gamma \) in \( \mathcal{R} \), leading to the collimation of the electron beam \( \textbf{18} \), i.e., \( |v_{Fb}(q)| > |v_{F}(q)| \). This expression is even valid where \( t^2 \gg |\Gamma|^2 \). On the other hand for \( t^2 \ll |\Gamma|^2 \) we obtain \( v_{Fb} \approx t_{\gamma} v_F(1 - |\Gamma|^2)/T_\gamma \) leading to the vanishing of collimation at chiral angles \( |\Gamma|^2 / (1 - |\Gamma|^2) \ll |\tau_{\gamma}| \ll (1 - |\Gamma|^2) \). For even smaller \( \tau_{\gamma} \) we obtain collimation again.

In Fig. \( \textbf{1} \) we see how the energy bands oscillate, in accordance with Eq. \( \textbf{9} \) for \( q \leq T_\gamma / \hbar v_F \), thus forming band SL valleys. The central valley possesses a true Dirac point at \( q = 0 \). The SL side valleys have then a minimum at \( \sin^2(\tilde{q} d/2) = 0 \). Within the SL valleys, electrons travel either to the left (right) for \( \partial \epsilon_s / \partial q < 0 \) (\( \partial \epsilon_s / \partial q > 0 \)). The number of side valleys can be read of from \( \textbf{4} \) as

FIG. 1: (Color online) Upper panel shows a NT with an overlying chiral electrical superlattice potential. Lower panel shows the two lowest energy bands \( (d = D) \) by solving Eq. \( \textbf{8} \) for \( \eta = 0 \) as a function of the rescaled axial quasi-momentum \( qd/2 \) for various chiral angles \( \gamma \) with \( Vd/2\hbar v_F = 5 \) (left panel) and various chiral potentials \( Vd/2\hbar v_F \) with \( \tau_{\gamma} = 1 \) (right panel). Note that the dotted curve in the right panel crosses the x-axis exactly only at \( q = 0 \).
2m_1 with m_1 = [\tau, Vd/T, \hbar v_F 2\pi].

For SLs with wavevector in exact axial direction we can read off the physics from the chiral case by choosing \( \hat{q} \rightarrow k, \tau_\gamma = \eta = 0 \) where d is now the wavelength of the SL potential in axial direction with quasimomentum k.

The wavevector q in the circumferential direction is quantized by q = 2m_1/D due to the periodic boundary conditions of the wavefunctions. We point out that also the wavefunctions Eqs. (11), (12), and the considerations below Eqs. (11), (13) are still valid with the additional replacements k_x \rightarrow k_y and x \rightarrow y. Eq. (9) delivers that the energy bands are separated by \( \hbar v_F \Gamma \) which means that the energy spacing between the energy bands goes to zero for infinite potential strength. From Eq. (9) we have v \rightarrow v_F for Vd/\hbar v_F \rightarrow \infty where for the lowest band, i.e. q = 0, v \rightarrow v_F even for finite potentials Vd/\hbar v_F.

Next, we determine the eigenvectors \( v^a \) of the matrix \( \Lambda(d) \). These are given by \( v^a = \frac{1}{N_\Lambda}[(a+i \sin(q+\hat{q}d))/b, 1]^T \) with

\[
a = \left[ qd_2 \cos(\alpha_1) \frac{\sin(\alpha_2)}{\alpha_2} + qd_1 \cos(\alpha_2) \frac{\sin(\alpha_1)}{\alpha_1} \right] \frac{1}{\Gamma^2},
\]

\[
b = \left[ k_2 d_2 \cos(\alpha_1) \frac{\sin(\alpha_2)}{\alpha_2} + k_1 d_1 \cos(\alpha_2) \frac{\sin(\alpha_1)}{\alpha_1} \right] \frac{i}{1 - it_\gamma},
\]

\[
- i \frac{\sin(\alpha_1) \sin(\alpha_2)}{\alpha_1 \alpha_2} \frac{d_1 d_2}{T^2} \frac{k - k_2}{1 - it_\gamma},
\]

and \( N_\Lambda \) is a normalization factor. The eigenfunction \( u^a(x, q) \) of the full Hamiltonian \( H_K \) is then given by \( u^a(x, q) = \langle \cos[\alpha_0(x)]I + \sin[\alpha_0(x)]/\alpha_0(x) \rangle M(v) v^a \) for \( x < d/2 \). Eq. (11) leads to \( u^a(x, q)e^{ik_x x} \langle u^{-a}(x, -q) \rangle = 0 \) where we used the abbreviation \( \langle u^a(x, q) \rangle e^{ik_x x} \langle u^{-a}(x, -q) \rangle = \int_0^d dx \langle u^a(x, q) \rangle e^{ik_x x} \langle u^{-a}(x, -q) \rangle \) for the \( \Gamma \) regime.

Here I is the identity matrix and \( \sigma_x, \sigma_y, \Gamma \) the spin matrices. The wavevector of the phonons or impurities is denoted by \( k_x \). This is a generalization of the results that inner-valley backward impurity scattering in Refs. [19, 20] used the abbreviation \( \hat{q}d \rightarrow \hat{q}d + \hat{q} \). Finally, we mention that for general chiral potentials \( V(x) \) leading effectively to the \( \sim q^2 \) correction factor in \( \alpha_0 \).

For large chiral angle \( |\tau_\gamma| \geq 1 \), for \( \langle qd^2/2 \rangle \ll 0 \), at large chiral angle \( \tau_\gamma \geq 1 \), for the \( \langle qd^2/2 \rangle \ll 4T^4 \sin(qd^2/2) \) and \( \langle qd^2/2 \rangle \ll 4T^4 \sin(qd^2/2) \) which is the relevant regime for transport at high applied bias voltages. We obtain

\[
|\langle u^a(x, q) |e^{ik_x x} |u^a(x, q') \rangle|^2 \approx (A_0^2)^2 \delta_{k_x, 0} \delta_{k_y, 0} \delta_{d, 0} \delta_{k_z} \rho \frac{1}{2} \sum_{j=1}^{m_2} \delta_{k_x, d, j} \approx 2|Vd/2\pi |Vd/2\pi v_F T \Gamma \},
\]

where \( (A_0^2)^2 \approx 0 \) and \( (A_1^2)^2 \approx 1 \). Here we introduced the abbreviation \( k_x = k_z - \hat{q}^\prime + \hat{q} \). Note that we used in (13) the approximation that \( \alpha_0(d_i) \approx d_i |V_i|/\hbar v_F T \Gamma \) valid for the majority of SL valleys.

For the symmetric two-step potential [11] we have \( m_2 = 1 \) and \( V_i = V \) in (13). We generalized in (13) our results to a chain of symmetric two-step potentials with \( d_1 = d_2 = d/2m_2 \) of potential heights \( V_i \) where we assume the potential heights are separated considerably \( \ll 2Vd/2\pi v_F T \Gamma \) \( \neq 0 \) for \( i \neq j \). This restriction implies that the number of different phonons taking part in an electron-phonon scattering process is maximal. Eq. (13) delivers that for every phonon type of certain momentum the scattering probability is \( \sim 1/2m_2 \) smaller than in the case of no existing chiral potential [12]. By using (12) we obtain for general step potentials within the same approximation used in (13) \( \sum_{k_x} |\langle u^a(x, q) |e^{ik_x x} |u^a(x, q') \rangle|^2 \approx 1 \) for \( \sigma = \sigma_x \)URL and zero for \( \sigma \in \{ \sigma_y, \sigma_I \} \). This shows with the help of the discussion in the second paragraph, that the considered chain of symmetric two-step potentials should give the best transport results over all step potentials and that even a general step potential should show an enhanced conductivity compared to the pristine NT.

The number of SL valleys for a chain of two-step potentials is now \( m_1 = [\tau, \min |V_i|/\hbar v_F T \Gamma] \) which can be read off from Eqs. (4) and (13) as in the case of the symmetric two-step potential. Here we denote \( \min |V_i| \) as the minimum of all \( V_i \)'s. Finally, we mention that for the forward scattering amplitudes, i.e. \( \partial_q \sin(qd^2/2) \leq 0 \)
scattering mechanism in this case \cite{5, 6}. We now have phonon backward scattering is the only relevant phonon-in the corresponding expressions \cite{21}. Zone boundary of the \( A \) valley by using the substitution \( K \) \( \rightarrow -K \) for a NT lying on a substrate without chiral potential which is equal to the number of different phonon species taking part in a backward scattering process.

In the following, we assume that higher bands do not contribute to the conductivity so that we have \( \hbar v_F T_2 \approx \epsilon U \) (\( \hbar v_F T_2 \approx \epsilon U \)) for wavectors of the SL out of (exact in) axial direction. For large enough applied bias voltages \( \epsilon U \gg |\epsilon_{s}(q_i)| \) where \( q_i \) is defined by \( \sin(q_i d/2) = 0 \). For \( q_i^2 \ll T_2^2(\min|V_j|d/\hbar v_F)^2 \) and large chirality, i.e. \( \tau_{\gamma} \gtrsim 1 \), we obtain the following idealized band system: We have one central SL band with dispersion \( \epsilon(k) \approx \pm \hbar v_F|k| \) and 2\( m \)SL sidebands with momentum shifted dispersion \( \epsilon(k) \approx \pm \lim_{k_0 \to 0} \hbar v_F \sqrt{k^2 + k_0^2} \). Phonons of \( 2m \) \( \nu \) types contribute to electron-phonon backward scattering with scattering times \( 2\nu \tau_{\nu \tau} \). Here \( \nu \) stands for \( \Gamma \) for longitudinal \( E_2 \) zone-center scattering or \( K \) for \( A^\prime \) zone boundary phonon scattering \cite{5, 6}. \( \tau_{\nu \tau} \) is the corresponding electron-phonon scattering time without chiral potential. We can simplify our calculation by using the same phonon velocity \( v_{\nu \tau} \) of the system without SL for all type of optical phonons. This is justified by the fact that our results do not depend much on the specific velocity value since the phonon mean free path is much smaller than the NT length as we have verified numerically.

It is enough to consider only forward scattering between the central SL valley and the 2\( m \) SL side valleys mediated by transversal optical \( \Gamma \) phonons with scattering time \( \tau_{\nu \tau} \) \cite{5, 6} where we use calculation methods established in Ref. \cite{23} for forward scattering. At low voltages \( U \approx 0.17V \), quasi-elastic scattering is relevant and we take it into account in our numerical calculations by inner SL valley scattering. This approximations is exact for voltages lower than the SL side valley energy gap. We can simplify even further the model to an effective two-valley model with one central SL valley and one side valley by using the approximation of periodic boundary conditions for the positions of the potential valleys in momentum space.

In Fig. 2, we show our results for the conductance, the differential conductance, and the position and energy averaged phonon number \( \tau_{\nu \tau} \) for certain \( (m_1, m_2) \) values and lengths \( L \). Here \( \nu \) mediates the inner SL valley scattering. Note that an upper limit for \( 2m_1, 2m_2 \) is given by the number of excitable circumferential phonons, i.e., \( 2m_1, 2m_2 \leq d/3a \) where \( a \) is the NT interatomic distance \( a \approx 1.42A \). We obtain a strong increase in the absolute conductance and differential conductance at high voltages \( (U \approx 2V) \) as a function of \( m_1 \) and \( m_2 \) while \( \tau_{\nu \tau} \) is strongly decreasing. The reason for an increase of the conductance for larger \( m_1 \) values and fixed \( m_2 \) comes mainly from the fact that due to the band edges of the side valleys scattering from the central SL valley to the SL side-valleys is effectively forward. The backscattering 
to the central valley is accomplished then by a number of different phonons in contrast to the system without chiral potential. The growth of the conductance as a function of $m_1$ is then seen from our discussion in the second paragraph which also leads to the explanation of the conductance increase as a function of $m_2$.

Summarizing, we have shown that large chiral unidirectional superlattice potentials in metallic NTs should lead to a large increase of the conductance, the differential conductance, and to a decrease of the optical phonon temperature at high voltage. We have shown this explicitly for a chain-like SL potential with symmetric steps. This kind of SL potential leads to the best transport results over all step potentials. Nevertheless, the main effect should be also observed for at least other SL step potentials with strong chirality. The effect arises from an increased number of phonons with different momenta but lower electron-phonon scattering probabilities contributing to the electron-phonon scattering process. As a result of our findings we expect an increase of the applicability of carbon NTs as metallic wires.

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