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Negative differential conductivity in conducting carbon nanotubes

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Abstract. A theoretical model and computations of the $I-V$ characteristics of long carbon nanotubes in a strong axial dc-fields at room temperatures have been presented. Negative differential conductivity has been predicted. It has been shown that $|\mathrm{d}I/\mathrm{d}V|$ for metal carbon nanotubes in the region of the negative differential conductivity significantly exceeds corresponding values for semiconducting ones. The predicted effect makes possible the design of wave-generating nanotube-based diodes for submillimeter and infrared ranges.

Since the discovery by Iijima [1] of carbon nanotubes (CNs), a great deal of interest has been focused on these quasi-one-dimensional monomolecular structures because of their unique physical properties (mechanical, electrical, optical, etc.) and the rapid experimental progress in the controlled preparation. Processes of electron transport in strong external fields when nonlinear effects are constitutive are of a great interest for potential applications in nanoelectronics and for experimental diagnostic of CN themselves.

In this report we report a theoretical phenomenological analysis of the $I-$ characteristics of CNs at room temperatures, when $k_{\mathrm{B}}T > \mathcal{E}_c$, $\Delta\mathcal{E}$. In our case, the current is produced by free charge carriers — quasiparticles which are π-electrons moving in the field of the crystalline lattice. The nonlinearity of the $I-V$ characteristic appears due to the nonlinear properties of the quasiparticle gas. We investigate the *negative differential conductivity* (NDC) $\mathrm{d}I/\mathrm{d}V < 0$ in CNs in a certain range of the field strength, predicted in [2].

Let us consider an undoped single-wall achiral CN $(m,0)$ or (m,m) exposed to a homogeneous axial dc-field E_z, $E_z = V/L$, where V is the voltage between the CN ends. We shall apply the semi-classical approximation considering the motion of π-electrons as a classical motion of free quasi-particles with dispersion law extracted from the quantum theory. With the account to the hexagonal crystalline structure of CNs, the tight-binding approximation gives [3]:

$$\mathcal{E}_s(p_z) = \pm\gamma_0\left[1 + 4\cos(ap_z)\cos\left(\frac{a}{\sqrt{3}}s\Delta p_\phi\right) + 4\cos^2\left(\frac{a}{\sqrt{3}}s\Delta p_\phi\right)\right]^{1/2} \qquad (1)$$

for the zigzag CNs and

$$\mathcal{E}_s(p_z) = \pm\gamma_0\left[1 + 4\cos(as\Delta p_\phi)\cos\left(\frac{a}{\sqrt{3}}p_z\right) + 4\cos^2\left(\frac{a}{\sqrt{3}}p_z\right)\right]^{1/2} \qquad (2)$$

for the armchair CNs. Here $\gamma_0 \sim 3.0$ eV is the overlapping integral, $a = 3b/2\hbar$, $b = 1.42$ Å is the C-C bond length. The $-$ and $+$ signs correspond to the valence and conduction bands, respectively. In view of the transverse quantization of the quasi-momentum, its transverse component can take m discrete values, $p_\phi = s\Delta p_\phi = \pi\sqrt{3}\,s/am$ $(s = 1, \ldots, m)$ and we used $\mathcal{E}(s\Delta p_\phi, p_z) \equiv \mathcal{E}_s(p_z)$ in both equations. As different from p_ϕ, we assume p_z

continuously varying within the range $0 \leq p_z \leq 2\pi/a$ what corresponds to the model of infinitely long CN ($L = \infty$). This model is applicable to the case under consideration because we are restricted to temperatures and/or voltages well above the level spacing [4].

The motion of quasi-particles in an external axial electric dc-field is described by the Boltzmann kinetic equation

$$eE_z \frac{\partial f(\boldsymbol{p})}{\partial p_z} = -\frac{1}{\tau}[f(\boldsymbol{p}) - F(\boldsymbol{p})], \tag{3}$$

where e is the electron charge, $F(\boldsymbol{p})$ is the equilibrium Fermi distribution function and τ is the relaxation time. The relaxation term of the equation (3) describes the electron–phonon scattering [5, 6], electron–electron collisions etc.

Utilizing the method originally developed in the theory of quantum semiconductor superlattices we can construct an exact solution of kinetic equation (3) without assuming the electric field to be weak [2].

Then in view of Eqs. (1)–(3) one can obtain [2]

$$j_z(E_z) = -\frac{8e\gamma_0}{\sqrt{3}\hbar bm} \sum_{r=1}^{\infty} \frac{r^2\Omega\tau}{1+(r\Omega\tau)^2} \sum_{s=1}^{m} F_{rs}\mathcal{E}_{rs}. \tag{4}$$

Here $\Omega = aeE_z$ for the zigzag CNs and $\Omega = aeE_z/\sqrt{3}$ for the armchair ones is the Stark frequency. This equation states the basis for the evaluation of $I-V$ characteristics. Let us estimate the restrictions to the theoretical approach being developed. As it has been stated above, the quasi-particles motion is described classically by Boltzmann equation (3). It imposes the limitation on the external electric field strength: $|E_z| < \gamma_0/2eR$ [2]. The Coulomb electron–electron interaction has been also left out of account in our analysis. The role of this mechanism as applied to CNs was discussed in [2].

The $I-V$ characteristics obtained via numerical calculation of Eq. (4) are presented in the right panel of Fig. 1 for the metal zigzag CNs and in the left one for the armchair CNs ($m \neq 3q$) zigzag CNs. The figures show the linear dependence of j_z on E_z at weak strengths of the external field; it corresponds to the region of ohmic conductivity. As E_z increases, the value $\partial j_z/\partial E_z$ growth smaller and at $E_z = E_z^{(\max)}$ the current density reaches the maximum value $j_z^{\max}$. Further increase of E_z results in the decrease of j_z. At small m the magnitudes of $E_z^{(\max)}$ and $j_z^{\max}$ for the armchair CNs turn out to be less than for zigzag CNs with similar radius by the factor approximately 2. As different from the zigzag CNs, the increase of m leads to the $E_z^{(\max)}$ growing up, and $I-V$ curves for zigzag and armchair CNs become practically identical at $R > 20$ nm. Thus, we predict the region with the negative differential conductivity $\partial j_z/\partial E_z < 0$, in the $I-V$ characteristics of CNs.

The external field strength $E_z^{(\max)} \approx 3.2 \cdot 10^3$ V/cm for the NDC region appears to be unexpectedly weak because the nonlinearity in the structure under consideration is determined by the value of aE_z; quantum superlattices with periods about 10^{-6} cm [8], much larger than b, show approximately the same fields for the NDC manifestation. It means that the nonlinearity in CNs is much higher than in superlattices. To explain this fact let us compare the mechanisms of the nonlinear conductivity in CNs and in the superlattices. The quantum superlattices are formed by alternating plain layers of different semiconducting materials, while the latteral superlattices consist of 1D chains of identical and identically coupled GaAs/AlGaAs quantum dots [8]. Both these structures are characterized by the dispersion law $\mathcal{E}(\boldsymbol{p}) = \Delta[1-\cos(\tilde{a}p_z)]$, with Δ as the overlapping integral and $\tilde{a} = 2a/3$.

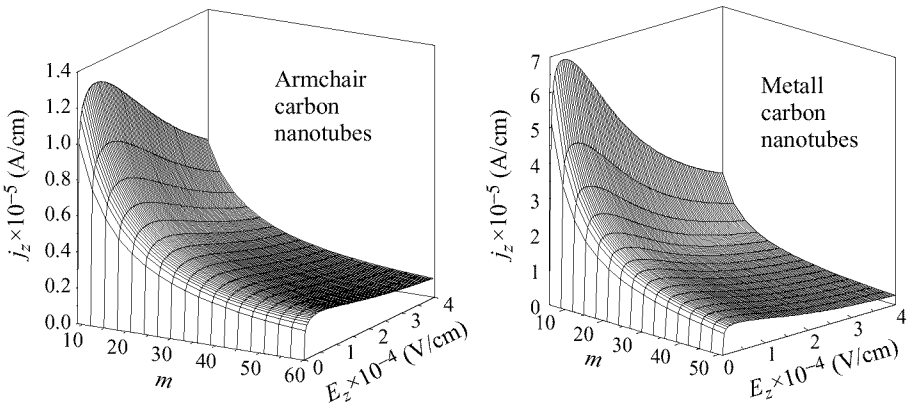

Fig. 1. $I-V$ curves for armchair (left panel) and metal zigzag (right panel) carbon nanotubes, $T = 287.5$ K, $\tau = 3 \cdot 10^{-12}$.

Applying the method described above to this dispersion law, one can obtain the Esaki–Tsu relation [7] $j_z(E_z) = \sigma_{zz} E_z/(1+\Omega^2\tau^2)$ instead of Eq. (4). Here $\sigma_{zz} = \lim_{E_z \to 0}(\partial j_z/\partial E_z)$ is the linear conductivity. Comparing two equations for the current density we can conclude that the specific peculiarity of the CNs is the presence of the *high Stark components* (summation with respect to r in Eq. (4)).

It has been shown that the electron motion in dc-field can be described as the oscillations of an ensembles of effective harmonic oscillators (Stark components) with the frequencies $r\Omega$. The full current is a superposition of partial currents of the Stark components. Their electrical field strength corresponding to maximum current of r-th Stark component decreases with r as r^{-1} while our calculations shows that oscillator strength of these component decreases slowly. This is due to the hexagonal crystalline structure of CNs reflected in dispersion laws (1) and (2). The number the unneglectable components is 70–150 for metal and 200–300 for semiconducting CNs. As a result, the role of the high Stark components in CNs is essential and the integral nonlinearity of the CNs is much higher than in superlattices [8].

Note that the NDC provides the current instability. It can be expected that simultaneously applied dc- and ac-fields will result in the dynamic electron localization (which is the nonlinear phase of the instability) and in the 2D analogue of the self-induced transparency, like it takes a place in the semiconducting superlattices. The above mentioned effects are responsible for the absolute negative conductivity which thus is predicted to be exhibited in CNs. It must result in the appearance of the absolute negative conductivity zones and active properties of CNs providing a potentiality for the design of generative nanodiodes in microwave and infrared ranges. Such a possibility relates to both single CNs and CN ropes.

The NDC effect was also predicted in Ref. [9] for the CN-junctions generated in the result of different ways of doping the sides of the tubes or via the applying an external potential difference between them. The comparison of physical mechanisms of the NDC in [9] and [2] is actual. In [9] the electric field is localized in the narrow region of the junction while in [2] it is homogeniously allocated along the CN. That is why the field strength in [9] is much higher under the same potential. In [9] the NDC was obtained for

the junctions based on metal CNs only, while [2] also contains the prediction of the NDC in semiconducting CNs, the effect being much weaker for them. The value of $E_z^{(\max)}$ for armchair CNs with small radius is approximately half as great than that for metal zigzag CNs with similar radius. This result was obtained in both papers. Thus one can come to a conclusion that physical mechanisms in [9] and [2] are close. However, it is necessary to note that the $I-V$ curves in [9], as different from [2], are unsymmetric with respect to the transformation $V \to -V$.

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References

[1] S. Iijima, *Nature* (London) **354**, 56 (1991).

[2] Ant. S. Maksimenko and G. Ya. Slepyan, *Phys. Rev. Lett* **84**, 362 (2000).

[3] M. F. Lin and K. W.-K. Shung, *Phys. Rev. B* **52**, 8423 (1995).

[4] C. Kane, L. Balents and M. P. A. Fisher, *Phys. Rev. Lett.* **79**, 5086 (1997).

[5] R. A. Jishi, M. S. Dresselhaus, and G. Dresselhaus, *Phys. Rev. B* **48**, 11385 (1993).

[6] C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **78**, 1932 (1997); C. L. Kane *et al.*, *Europhys. Lett.* **41**, 683 (1998).

[7] L. Esaki and R. Tsu, *IBM J. Res. Dev.* **14**, 61 (1970).

[8] E. P. Dudin, A. A. Zharov, and A. A. Ignatov, *J. Exp. Theor. Phys.* **87**, 1226 (1998).

[9] A. A. Farajian, K. Estarjani and Y. Kawazoe, *Phys. Rev. Lett.* **82**, 5084 (1999).