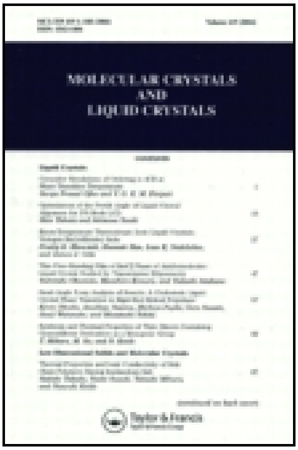

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Chirality-Dependent Resistivity in Carbon Nanotubes

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Chirality-Dependent Resistivity in Carbon Nanotubes

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The phonon-mediated resistivity is calculated for metallic carbon nanotubes based on a continuum model for electrons and phonons. In armchair nanotubes, only twisting modes contribute to the resistivity, while both stretching and breathing modes are important in zigzag nanotubes. The resistivity shows chirality dependence at low temperatures where breathing modes are not populated but becomes independent of the chirality at high temperatures.

Keywords: carbon nanotubes; electron-phonon scattering; resistivity

1. INTRODUCTION

Since the discovery of carbon nanotubes (CN's) [1], quite a number of studies have been reported on their electronic properties and it turned out that CN's become metallic or semiconducting dependent on their structure [2]. Quite recently, it was shown theoretically that there is no backscattering for impurity potentials with a range larger than the lattice spacing in metallic CN's [3]. A conductance quantization was observed for multi-wall CN's [4]. In this paper we focus on electron-phonon scattering as the main origin of resistivity and reveal its chirality dependence.

We introduce continuum models which describe low-energy excitations both for electrons and for phonons. The electronic properties of CN's have been understood by those of the graphite plane using a periodic boundary condition [5]. On the other hand, the phonon modes of nanotubes are not simply given by the zone-folded modes of planes because they fail to give breathing modes [6].

2. MODEL

Metallic CN's have two Fermi points corresponding to the K and K' points in the graphite plane and the low-energy electronic properties around each

Fermi point are described by a matrix $\boldsymbol{k}\cdot\boldsymbol{p}$ equation [5] which is the same as Weyl's equation for the neutrino and is given in the cylindrical coordinates (r, θ, z) by

$$\epsilon \begin{pmatrix} F_A(\theta, z) \\ F_B(\theta, z) \end{pmatrix} = \hbar v_F \begin{pmatrix} 0 & -iR^{-1}\partial_\theta - \partial_z \\ -iR^{-1}\partial_\theta + \partial_z & 0 \end{pmatrix} \begin{pmatrix} F_A(\theta, z) \\ F_B(\theta, z) \end{pmatrix}, \tag{2.1}$$

where v_F is the Fermi velocity, $\hbar v_F = 6.46$ eVÅ, and R is the radius of the CN. We use the abbreviation for differential operators as $\partial_\theta = \partial/\partial\theta$, etc. Eigenstates of the Hamiltonian (2.1) are given by

$$\boldsymbol{F}(\theta, z) = \frac{1}{\sqrt{2\pi RA}} \begin{pmatrix} 1 \\ \pm e^{i\theta_k} \end{pmatrix} e^{i(n\theta + k_z z)}, \tag{2.2}$$

where A is the length of the CN, n is an integer, and $e^{i\theta_k} = (k_\theta + ik_z)/|k_\theta + ik_z|$ with $k_\theta = n/R$, and the eigenenergy is equal to $\pm\hbar v_F\sqrt{k_\theta^2 + k_z^2}$.

For acoustic phonons of nanotubes, we introduce the Lagrangian of the following continuum elastic model using cylindrical coordinates:

$$\begin{aligned} L_{ph} &= K[\boldsymbol{u}] - U[\boldsymbol{u}], \\ K[\boldsymbol{u}] &= \int dS\, \frac{M}{2}\Big[(\partial_t u_r)^2 + (\partial_t u_\theta)^2 + (\partial_t u_z)^2\Big], \\ U[\boldsymbol{u}] &= \int dS\, \frac{1}{2}\Big[B\big(u_{\theta\theta} + u_{zz}\big)^2 + \mu\Big(\big[u_{\theta\theta} - u_{zz}\big]^2 + 4u_{\theta z}^2\Big)\Big], \end{aligned} \tag{2.3}$$

with the displacement vector $\boldsymbol{u} = (u_r(\theta, z), u_\theta(\theta, z), u_z(\theta, z))$ and the strain tensors $u_{\theta\theta} = R^{-1}(\partial_\theta u_\theta + u_r)$, $u_{zz} = \partial_z u_z$, and $2u_{\theta z} = \partial_z u_\theta + R^{-1}\partial_\theta u_z$. The integral should be executed all over the surface of a CN. The parameters B and μ denote the bulk modulus and the shear modulus for a graphite sheet because this model describes phonons of a graphite sheet in the infinite R limit. The mass density M is the carbon mass per unit area, $M = 9.66 \times 10^{-7}$ kg/m^2.

For $q_\theta = 0$, the eigen equation becomes

$$M\omega^2 \begin{pmatrix} u_r \\ u_\theta \\ u_z \end{pmatrix} = \begin{pmatrix} (B+\mu)R^{-2} & 0 & (B-\mu)R^{-1}iq_z \\ 0 & \mu q_z^2 & 0 \\ -(B-\mu)R^{-1}iq_z & 0 & (B+\mu)q_z^2 \end{pmatrix} \begin{pmatrix} u_r \\ u_\theta \\ u_z \end{pmatrix}, \tag{2.4}$$

which has three eigenmodes called twisting, stretching, and breathing modes. The twisting mode is made of pure circumference-directional deformation and its velocity v_t is equal to that of the TA mode of a graphite sheet, $v_t = v_T^G = \sqrt{\mu/M}$. In the long wavelength limit $|q_z R| \ll 1$, the deformation in the nanotube-axis direction generates stretching modes. Its velocity $v_s = \sqrt{4B\mu/[(B+\mu)M]}$ is usually smaller than that of the LA mode of the graphite $v_L^G = \sqrt{(B+\mu)/M}$. The radial deformation generates a breathing mode with a frequency $\omega_b = \sqrt{(B+\mu)/M}/R$, which is inversely proportional to the radius R of the CN. We set $v_L^G = 21.1$ km/s and $v_T^G = 15.0$ km/s, and we obtain $v_s = 21.1$ km/s, $v_t = 15.0$ km/s, and $\hbar\omega_b = 2.04 \times 10^{-2}$ eV, or 237K for the [10, 10] armchair CN with $R = 6.785$ Å. These values show good agreement with recent results by Saito et al. [7] and can never be reproduced by a zone-folding method.

Interactions of an electron with acoustic phonons are usually described by a deformation potential appearing as a diagonal energy shift in the $\boldsymbol{k}\cdot\boldsymbol{p}$ equation. There can be an off-diagonal term due to local modification of the band structure caused by acoustic phonons. Within a tight-binding model this can be described by a deformation of a transfer integral between nearest-neighbor sites [8]. Except at temperatures much higher than room temperature, phonons connecting different Fermi points (K and K' points) [9] are hardly populated and their effects can safely be neglected. The electron-phonon interaction is described by the following matrix Hamiltonian:

$$\begin{aligned} V_{el-ph} &= \begin{pmatrix} V_1 & V_2 \\ V_2^+ & V_1 \end{pmatrix}, \\ V_1 &= g_1 \left(u_{\theta\theta} + u_{zz}\right), \\ V_2 &= g_2 e^{i3\eta} \left(u_{\theta\theta} - u_{zz} + 2iu_{\theta z}\right), \end{aligned} \tag{2.5}$$

where η is the chiral angle which is equal to 0 for zigzag nanotubes and $\pi/6$ for armchair nanotubes.

The parameter g_1 is chosen as the known deformation potential of graphite, i.e., $g_1 \sim 30$ eV [10]. As for g_2, we need microscopic information on phonons as well as the derivative of the transfer integral with respect to the distance r between two carbon atoms A and B, $q_0 = -\gamma(b)^{-1}\partial_r\gamma(r)|_{r=b}$, where $\gamma(r)$ is the transfer integral and b is the equilibrium bond length. This parameter was estimated as $g_2 = \hbar v_F q_0/2$ by assuming $\boldsymbol{u}_A(\boldsymbol{R}_n^A) = \boldsymbol{u}(\boldsymbol{R}_n^A)$ and $\boldsymbol{u}_B(\boldsymbol{R}_n^B) = \boldsymbol{u}(\boldsymbol{R}_n^B)$, where $\boldsymbol{u}(\boldsymbol{R})$ is the lattice displacement obtained in a usual elastic model [8,11], and $\boldsymbol{u}_A(\boldsymbol{R}_n^A)$ and $\boldsymbol{u}_B(\boldsymbol{R}_n^B)$ are actual displacements of carbon A and B atoms at sites $\boldsymbol{R}_n^A$ and $\boldsymbol{R}_n^B$, respectively. This procedure is not correct, however. Here, we use a microscopic valence-force-field model and have $g_2 = (\hbar v_F q_0 \mu)/(2B)$. We estimate g_2 to be 8.2 eV with $q_0 = 2.5$ Å^{-1} [8].

3. RESISTIVITY

Around the Fermi point, only two modes with $k_\theta = 0$ and $k_z = \pm k$ with $k = |\varepsilon|/\hbar v_F$ play a role in transport. Therefore, the relaxation time τ

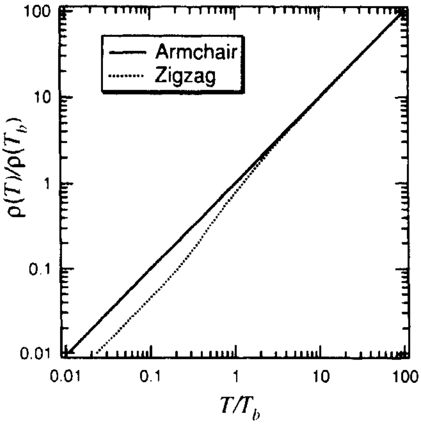

FIGURE 1 Temperature dependence of the resistivity of armchair (solid line) and zigzag (dotted line) nanotubes. The lines are plotted in units of $\rho(T_b)$ which is the resistivity of the armcahair nanotube at $T=T_b$, and T_b denotes the temperature of the breathing mode, $T_b=\hbar\omega_b/k_B$

is determined by the scattering rate between the two modes mentioned above via emission and absorption of phonons with $\boldsymbol{q}=(0,\pm 2k)$,

$$\begin{aligned}\frac{1}{\tau}=\frac{g_2^2}{2\pi RMv_F}\sum_l \frac{N_T[\omega_l(\boldsymbol{q})]}{\hbar\omega_l(\boldsymbol{q})}\\ \times\left|\Big(R^{-1}U_l^r(\boldsymbol{q})-i2kU_l^z(\boldsymbol{q})\Big)\cos(3\eta)-i2kU_l^\theta(\boldsymbol{q})\sin(3\eta)\right|^2,\end{aligned} \tag{3.1}$$

where $N_T(\omega)$ is the boson distribution function, $N_T(\omega)=1/(e^{\hbar\omega/(k_BT)}-1)$. In deriving Eq.(3.1) we have neglected the energy of acoustic phonons in comparison with that of electrons, which automatically leads to $N_T(\omega)\approx N_T(\omega)+1$. This approximation is justified because the Fermi velocity is much larger than phonon velocities. The resistivity is given by

$$\rho=\frac{h}{8e^2v_F\tau}, \tag{3.2}$$

with spin degeneracy and two Fermi points taken into consideration.

The above expression of the relaxation time shows that only the twisting mode is effective in armchair nanotubes ($\eta=\pi/6$). Under the condition that phonons are heavily populated, $N_T(\omega)\simeq k_BT/(\hbar\omega)$, we have

$$\rho_A(T)\simeq\frac{g_2^2}{2e^2\hbar v_F^2R\mu}k_BT. \tag{3.3}$$

This agrees with the previous result [11] except for the difference in the actual value of g_2.

On the other hand, the resistivity ρ_Z of zigzag nanotubes ($\eta = 0$) has contributions from the stretching mode and the breathing mode. Because the breathing mode has a finite energy gap, only the stretching mode contributes to the resistivity at temperatures lower than $T_b = \hbar\omega_b/k_B$. Therefore, we have

$$\rho_Z(T) = \frac{B}{B+\mu}\rho_A(T), \tag{3.4}$$

for $T \ll T_b$. The contributions from the breathing mode increase with temperature and in the high-temperature limit $T \gg T_b$ we have

$$\rho_Z(T) = \rho_A(T). \tag{3.5}$$

Thus, the resistivity shows a universal behavior, independent of chirality at temperatures much higher than T_b.

Figure 1 shows the temperature dependence of the resistivity of the armchair (solid line) and zigzag (dotted line) nanotubes with the same radius R. The resistivity of armchair nanotubes, ρ_A, shows a uniform linear dependence on temperature, while that of zigzag nanotubes shows a different behavior between the low and high temperature region, though it is proportional to temperature in both regions. At high temperatures the resistivity becomes independent of the chirality. All of these features can be understood from the discussion given above.

It is worth noting that τ is independent of g_1. This corresponds to the absence of backward scattering for impurities with a potential range larger than the lattice constant [3]. The situation changes drastically and the deformation potential starts to give rise to backscattering, when a magnetic field is applied perpendicular to the axis, which is likely to lead to a positive magnetoresistance. This will be discussed elsewhere.

The mean free path l_m of a CN with the radius R is estimated to be $194 \times R$ at room temperature and, for example, that of CN with $R = 50$ Å reaches 1 μm. This shows that a conductance quantization can be observed for CN's with large radius even at room temperature.

4. CONCLUSION

We have studied the temperature dependence of the resistivity due to low-energy acoustic phonon scattering based on a continuum model. The continuum model introduced for phonons reproduces low-energy modes without using a zone-folding method, and the electron-phonon interaction is dependent on the chirality of CN's. As a result, the resistivity, which is proportional to temperature, is dependent on the chirality at temperatures lower than the energy of the breathing mode. At higher temperatures, the chirality dependence of the resistivity disappears completely. It is quite possible that this crossover of the temperature dependence between low and high temperature regions is experimentally observable because the temperature corresponding to the breathing mode is easily accessible. We have, for example, $T_b = 237$ K for $[10, 10]$ armchair nanotubes.

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