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Abstract

Using the semiclassical approach we studied the thermoelectrical properties of a single-walled chiral carbon nanotubes (SWNTs). We predict a giant electrical power factor and hence proposed the use of carbon nanotubes as thermoelements for refrigeration.

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Modern research on thermoelectrics(TEs) started with Ioffe's observation that doped semiconductors were the best thermoelectrics[1] . He also proposed that TEs could be used to make solid state refrigerators. Research efforts have concentrated on improving the thermoelectric figure of merit, $Z = \alpha^2/\rho\chi$ of thermodevices; be they generators, thermocouples or refrigerators. α is the thermopower, ρ is the electrical resistivity, χ the thermal conductivity, and α^2/ρ is referred to as the electrical power factor.

Currently, all the established thermoelectric materials are semiconductors in which the thermal conductivity consists mainly of two contributions; a lattice and an electronic components. In general, the former is significantly the larger of the two. Solid state theory has provided theoretical models of the lattice thermal conductivity. Over the past four decades, research efforts have focused on its reduction. Unfortunately, these efforts have met with limited success owing to an accompanying degradation in electrical properties[2] . Recently, it has been shown that Z is strongly enhanced in quantum wells, superlattices and multiple potential barriers, due to the two-dimensional carrier confinement[3–6]. In [7] , Baladin and Wang predicted that Z can increase even further in quantum well structures with free-surface or rigid boundaries. This additional increase is due to spatial confinement of acoustic phonons and, the corresponding modification of their group velocities. Superlattices of semiconductors and semimetals are expensive for mass production, hence the need to search for new materials.

There has been a resurgence of interest in the study of the Rare-Earth compounds, because they have high Seebeck coefficient[8] . In [9] Rowe *et al*, studied the electrical resistivity and Seebeck coefficient of $YbAl_3$. Their preliminary results showed that $YbAl_3$ possesses an electrical power factor double those of the state of the art thermoelectrical materials based on Bi_2Te_3 alloys.

In this letter, we report a giant electrical power factor of a chiral carbon nanotube. We shall proceed as in [10, 11] , by considering an infinitely long chain of carbon atoms wrapped along a base helix, a model of single-walled carbon nanotubes(SWNTs). As stated in [10, 11] , the chief merit of this model is its analytical tractability, which readily yields physically interpretable results.

The problem is considered in a semiclassical approach by solving the Boltzmann kinetic equation for the distribution function which in the τ constant approximation is given as,

$$\begin{aligned} f(p) &= \tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right) f_o(p-eEt)dt + \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \\ &\cdot\left(\left[\varepsilon(p-eEt)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right) v(p-eEt)\frac{\partial f_o(p-eEt)}{\partial\varepsilon}, \end{aligned} \tag{1}$$

where $\varepsilon(p)$ is the energy of the electrons and μ is the chemical potential, whilst E is the constant applied electric field. T is the temperature, p is the electron dynamical momentum, τ is the electron relaxation time and e is the electron charge. Seeking the current density j in the form

$$\mathbf{j} = e\sum_p \mathbf{v}(p)f(p),$$

where $v(p)$ is the velocity of the electron, we use the method and conditions in [12] and quoted the results for axial j_z and circumferential j_c currents as follows

$$\begin{aligned} j_z &= \left(\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\right)\nabla_z\left(\frac{\mu}{e}-\phi\right) \\ &- \left\{\sigma_z(E)\frac{k}{e}\left(\frac{\varepsilon_o-\mu}{kT}-\Delta_z^*\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}+2-\Delta_s^*\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*}\right)\right. \\ &+ \left.\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left(\frac{\varepsilon_o-\mu}{kT}-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right)\right\}\nabla_z T \end{aligned} \tag{2}$$

$$\begin{aligned} j_c &= \left(\sigma_s(E)\sin\theta_h\cos\theta_h\right)\nabla_z\left(\frac{\mu}{e}-\phi\right)-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h \\ &\cdot\left(\frac{\varepsilon_o-\mu}{kT}-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right)\nabla_z T, \end{aligned} \tag{3}$$

where ϕ is the electrostatic potential. From eqns.(2) and (3), the electrical conductivities are given as

$$\sigma_{zz} = \sigma_z(E)+\sigma_s(E)\sin^2\theta_h \tag{4}$$

$$\sigma_{cz} = \sigma_s(E)\sin\theta_h\cos\theta_h \tag{5}$$

where,

$$\sigma_z(E) = \frac{n_o e^2 \Delta_z d_z^2 \tau I_1(\Delta_z^*)}{\hbar^2 \left(1+(\Omega_z\tau)^2\right) I_0(\Delta_z^*)};$$

$$\sigma_s(E) = \frac{n_o e^2 \Delta_s d_s^2 \tau I_1(\Delta_s^*)}{\hbar^2 \left(1+(\Omega_s\tau)^2\right) I_0(\Delta_s^*)};$$

$$\Omega_z = \frac{eE_z d_z}{\hbar};$$

$$\Omega_s = \frac{eE_s d_s}{\hbar};$$

$$\Delta_i^* = \frac{\Delta_i}{kT}, \ i = z, \ s.$$

The differential thermoelectric power α is defined as, the ratio

$$\frac{|\nabla\left(\frac{\mu}{e}-\phi\right)|}{|\nabla T|}$$

in an open circuit. Hence, of interest to us is thermoelectric power along the axial and circumferential directions, which are obtained from eqns.(2) and (3) as

$$\alpha_{zz} = \left[\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left\{\frac{\varepsilon_o-\mu}{kT} - \Delta_z^*\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)} + 2 - \Delta_s^*\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\right.$$
$$\left. + \frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left\{\frac{\varepsilon_o-\mu}{kT} - \Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\right] \tag{6}$$

$$\alpha_{cz} = \frac{k}{e}\left[\frac{\varepsilon_o-\mu}{kT} - \Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right] \tag{7}$$

The intention of this letter is to manifest the giant electrical power factor associated with single-walled chiral CNTs. We therefore, plotted the eletrical resistivity ρ, thermopower (Seebeck coefficient) α_z and the electrical power P against temperature T.

Figure1 shows the dependence of resistivity ρ against temperature T for $\Omega\tau = 1$, 2 and 3. We noted that ρ increases slowly at low temperatures up to 200K, and gradually increases at high temperatures. There is also a marked increase in resistivity as $\Omega\tau$ increases. This is to be expected because in high fields, interaction of carriers with the lattice and other impurities increases, and thus, increase resistivity. The values of resistivity noted in this work are very low compared with those of the known materials[8, 13].

The thermopower (Seebeck coefficient) α_z, as seen from figures 2 and 3, show remarkable features. It behaves as p-type semiconductor and then, gradually becomes semimetallic as we change the values of Δ_s from 0.015 eV through 0.018eV to 0.020eV for $\Delta_z = 0.024$ eV. As Δ_s increases to 0.027eV (Figure 3) we observe complete semimetallic behaviour. For more details of how α_z changes with increasing values of Δ_z see [12].

In fact the most intriguing fact is the electrical power factor P. As seen in figure 4, where P is plotted against T for values of $\Omega\tau = 1$, 2 and 3, we observed that P has the highest peak at low fields, and the peaks drop off fast as we increase $\Omega\tau$. In figure 5, we plotted P against T for different values of Δ_s ranging from 0.015eV through 0.018eV to 0.020eV for $\Delta_z = 0.027$eV. We observed that the highest peak occurs at 0.015eV, i.e. when Δ_s is small and it also falls off as Δ_s increases.

As seen from the graphs, P is measured not in μW/mK^2 but in W/mK^2 and the peaks occur around 100K. Compared with $YbAl_3$ material which is currently the preferred material[9] P is about 5 times bigger when we take the peak values to be 0.04 W/mK^2. In figures 6 and 7, we present three-dimensional plots of P against T and Δ_z, and α_z against T and Δ_z for $\Delta_s = 0.018$eV.

In conclusion, we predict a giant electrical power factor and therefore suggest the use of single-walled chiral CNTs as thermoelements for refrigeration.

Acknowledgements

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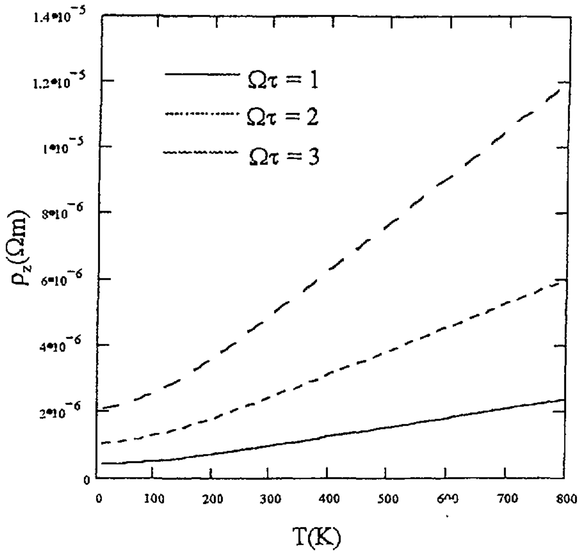


Figure 1. Dependence of resistivity ρ on temperature for $\Omega\tau = 1$, 2 and 3. $\Delta_z = 0.024$eV; $\Delta_s = 0.018$eV

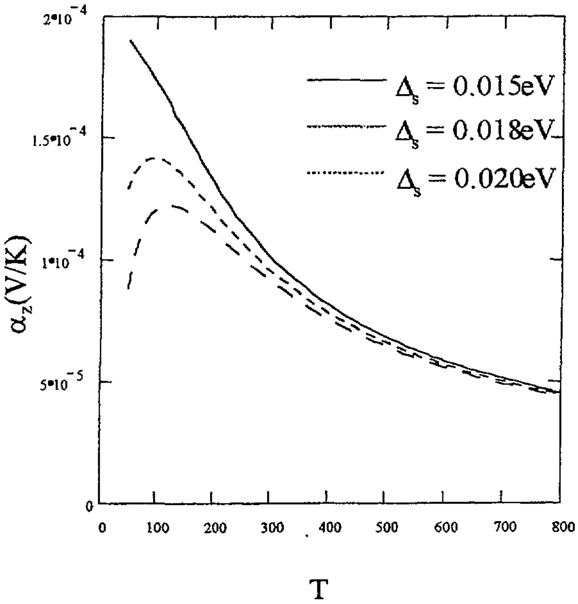


Figure 2. Dependence of thermopower α_z on temperature for $\Delta_s = 0.015$, 0.018 and 0.020eV; $\Delta_z = 0.024$eV

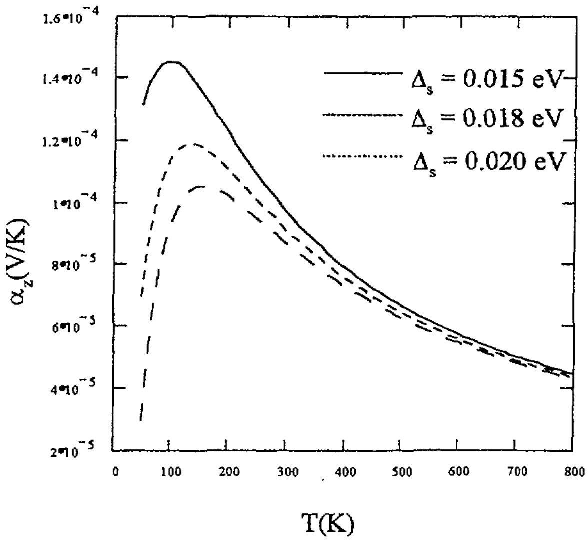


Figure 3. Dependence of thermopower α_z on temperature T for $\Delta_s = 0.015, 0.018$ and 0.020eV; $\Delta_z = 0.027$eV

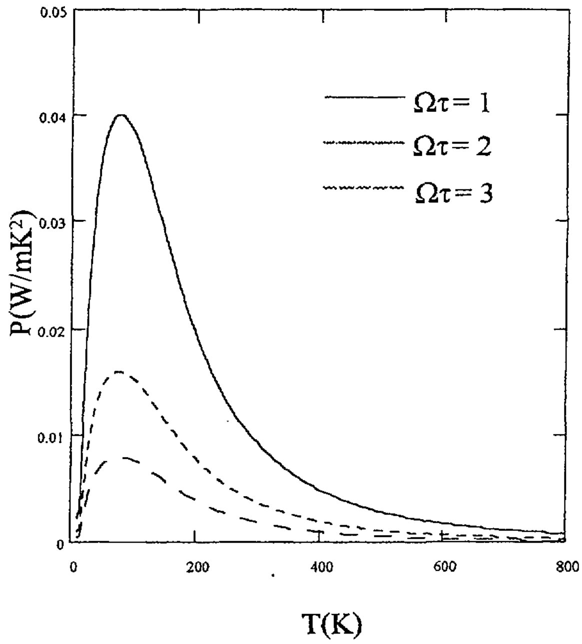


Figure 4. Dependence of power factor P on temperature T for $\Delta_s = 0.015, 0.018, 0.020$eV; $\Delta_z = 0.024$eV

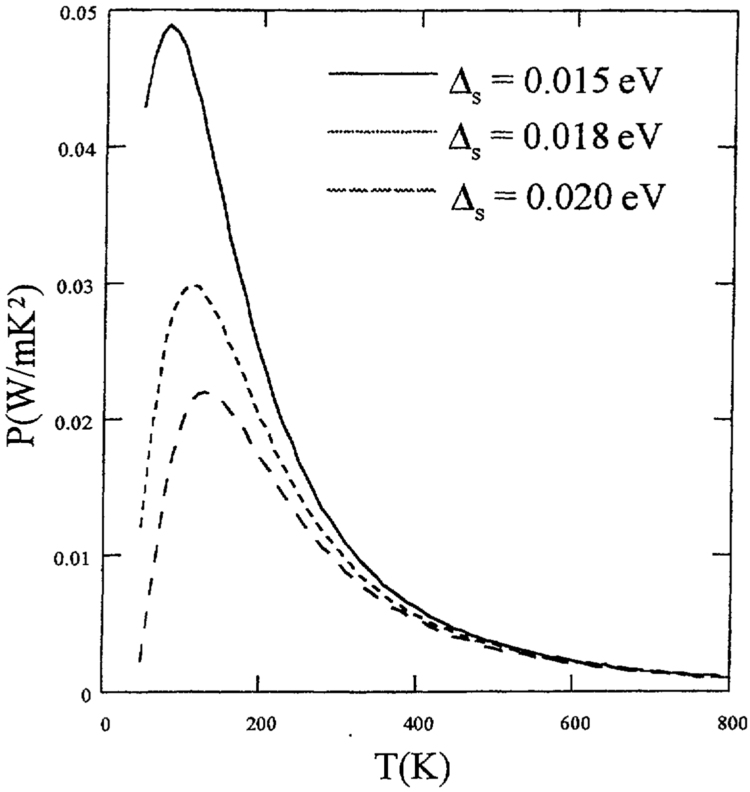
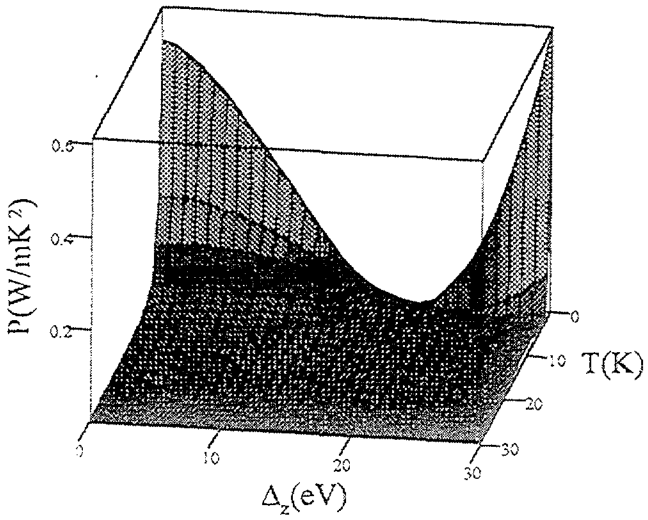
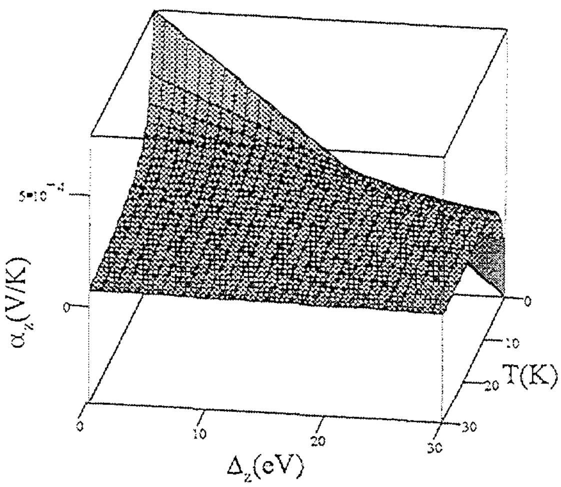


Figure 5. Dependence of power factor P on temperature T for $\Delta_s = 0.015, 0.018, 0.020$eV; $\Delta_z = 0.027$eV



P

Figure 6. Three-dimensional plot of power factor $P(T, \Delta_z)$ for $\Delta_s = 0.018$eV. Scale on T axis is 1 unit : 26Kand that on Δ_z axis is 1 unit : 1.3×10^{-3}eV



α

Figure 7. Three-demensional plots of thermopower $\alpha_z(T, \Delta)$ for $\Delta_s = 0.018$eV. Scale on T axis is 1 unit : 26Kand that on Δ_z axis is 1 unit : 1.3×10^{-3}eV