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Photo-Thermoelectric Effect Of Graphene Nanoribbon Nanodevice

Walid S. Mohamed, Mina D. Asham
Dept. of Basic Engineering Science
Faculty of Engineering, Benha University
Benha, Egypt
walidsol@yahoo.com, minadanial@yahoo.com

Adel H. Phillips
Dept. of Engineering Physics and Mathematics
Faculty of Engineering, Ain-Shams University
Cairo, Egypt
adel.phillips@gmail.com

***Abstract*—the thermoelectric effect of strained graphene nanoribbon nanodevice is investigated. This nanodevice is modeled as: A graphene nanoribbon is connected to two metallic leads. These two metallic leads operate as a source and drain. The conducting substance is the gate electrode in this three terminal nanodevice. Another metallic gate is used to govern the electrostatics and the switching of graphene nanoribbon channel. The substances at the graphene nanoribbon/ metal contact are controlled by the back gate. The Seebeck and Nernst *coefficients*, electronic thermal conductance, electrical conductance, figure of merit and the efficiency are computed at different temperature. Results show that both Seebeck coefficient and figure of merit of the present nanodevice are enhanced due to the induced tensile uniaxial strain. This is because of the reduced values of the electronic thermal conductance due to the induced tensile strain. So the present results show an enhancement of the thermoelectric properties of the present investigated nanodevice. As a consequence of our results, we might predict that the strained graphene nanoribbon is a promising nanomaterial for thermal to electrical energy conversion.**

Keywords—Seebeck and Nernst coefficients; electronic thermal conductance; figure of merit; thermoelectric efficiency; armchair and zigzag graphene nanoribbons.

I. INTRODUCTION

Direct energy conversion from thermal to electrical energy, based on thermoelectric effects, is attractive for applications in waste heat recovery and environmentally friendly refrigeration [1]. The energy conversion efficiency of thermoelectric devices is related to the thermoelectric figure of merit, which is proportional to the electrical conductivity, the square of the Seebeck coefficient, the temperature, and the inverse of thermal conductivity. Currently thermoelectric materials receive considerable attention [2] due to their ability to produce electricity from waste heat generated in, for example, power plants and refrigeration units. The efficiency of a thermoelectric material is characterized by the figure of merit.

Good thermoelectric devices at nanoscale are those where the heat dissipated or wasted is efficiently transformed into useful electricity and vice-versa [3]. The figure of merit ZT is a coefficient that quantifies the efficiency in the heat-to-electricity (electricity-to-heat) conversion process. When the heat is only carried out by electrons then the ZT is proportional to the square of the Seebeck (thermopower) coefficient or the ratio between the electrical and thermoelectrical linear conductance under the open-circuit condition.

Graphene nanoribbons (GNRs) are promising materials for nanoelectronics [4, 5].Graphene nanoribbons (GNRs), the narrow strips of graphene with few nanometers width, are particularly considered as a significant element for future nanoelectronics. GNRs exhibit several intriguing electronic [6], thermal [7] and mechanical [8] properties dominated by their geometry i.e., width or edge structure [9–11].In recent years, GNRs have been intensively investigated, including thermal transport properties, electronic transport properties as well as thermoelectric energy conversion [12–15]. It is well known that for the perfect GNRs, its thermal conductivity is large [1]. Thus, it is still considered to be very inefficient thermoelectric materials with very small the figure of merit and consequently very low thermoelectric efficiency. To increase the figure of merit, many ways to suppress the thermal conductivity have been predicted theoretically, including the edge disorder [16], defect-engineering [17]and antidot lattices [18,19].Moreover, the corresponding figure of merit can be enhanced by introducing randomly distributed hydrogen vacancies into completely hydrogenated GNRs [20]**.**The authors [21-23] show that tensile strain reduces the thermal conductivity of graphene nanoribbons which leads to enhanced values of the figure of merit of them and thermoelectric efficiency.

The quantum transport characteristics of graphene nanoribbon field effect transistor are investigated [24] under the influence of both the ac-field with different frequencies and magnetic field. The effect of an external tensile strain on the quantum transport characteristics of graphene nanoribbon was studied [24]. The aim of the present paper is to investigate the thermoelectric effect in graphene nanoribbon field effect transistor under the influence of tensile strain.

II. Theoretical Model

In this section, the thermoelectric parameters for the given investigated armchair and zigzag graphene nanoribbons nanodevice are expressed in terms of the tunneling probability, which has been derived by solving the Dirac equation [24] of the present studied nanodevice. The model of graphene nanoribbon is:

A graphene nanoribbon is connected to two metallic leads. These two metallic leads operate as a source and drain. The conducting substance is the gate electrode in this three terminal nanodevice. Another metallic gate is used to govern the electrostatics and the switching of graphene nanoribbon channel. The substances at the graphene nanoribbon/ metal contact are controlled by the back gate. The Dirac fermions charge carrier tunneling through the present investigated nanodevice is induced by an external applied ac-field which is given by:

$$V = V_{ac}\cos\omega t \tag{1}$$

where V_{ac} is the amplitude of the applied ac-field and ω is its frequency. The Seebeck coefficient, S, is given by [25, 26]:

$$S = \frac{1}{eT}\cdot\frac{\int dE\, f_{FD}(1-f_{FD})\Gamma_{withphotons}(E).(E-\mu)}{\int dE f_{FD}(1-f_{FD})\Gamma_{withphotond}(E)} \tag{2}$$

where f_{FD} is Fermi-Dirac distribution function, $\Gamma_{withphotons}(E)$ is the photon assisted tunneling probability [24] and μ is the electrochemical potential. The electronic thermal conductance, κ_e, is expressed in terms of the conductance, G(E), as [25,26]:

$$\kappa_e = L\cdot G(\mathrm{E})\cdot T \tag{3}$$

Where L is the Lorentz number for graphene nanoribbons and T is the temperature. The expression for L is [25,26]:

$$L = (k_B/e)^2\cdot\left[\left(\frac{3F_{\frac{3}{2}}}{F_{\frac{1}{2}}}\right)-\left(\frac{3F_{\frac{1}{2}}}{F_{-\frac{1}{2}}}\right)\right]^2 \tag{4}$$

Where k_B is Boltzmann constant, e is the electron charge and F_i is an integration of the reduced Fermi Dirac distribution function and it is:

$$F_i = F_i(\eta) = \int\frac{x^i dx}{e^{x-\eta}+1} \tag{5}$$

Where ζ is the band gap edge is given by:

$$\zeta = E_F \pm 0.5E_g \tag{6}$$

Where E_g is energy gap, E_F is Fermi energy. It must be noted that positive sign for conduction band and negative sign for valence band. After performing integration of above equation asymptotically for different $i = -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$ we get:

$$F_{\frac{-1}{2}}(\zeta) = \frac{2}{\sqrt{\pi}}\zeta^{\frac{1}{2}} \tag{7}$$

$$F_{\frac{1}{2}}(\zeta) = \frac{4}{3\sqrt{\pi}}\zeta^{\frac{3}{2}} \tag{8}$$

$$F_{\frac{3}{2}}(\zeta) = \frac{8}{15\sqrt{\pi}}\zeta^{\frac{5}{2}} \tag{9}$$

The thermoelectric figure of merit, ZT, of the present nanodevice is expressed as [27-29]:

$$ZT = \frac{S^2GT}{\kappa_{ph}+\kappa_e} \tag{10}$$

where κ_{ph} is the phonon contribution to thermal conductance. In the paper, we might neglect the phonon contribution to thermal conductance Eq.(10). This is because our calculations will be performed at very low temperature. It can be taken into consideration when we consider electron-phonon interaction and phonon drag. So, Eq.(10) will take the following form as:

$$ZT = \frac{S^2GT}{\kappa_e} \tag{11}$$

The Nernst coefficient, N_T, is expressed as [28,30]:

$$N_T = \frac{1}{8\pi k_B T^2}\int dE\, f_{FD}(1-f_{FD})\Gamma_{withphotons}(\mathrm{E})(E-\mu) \tag{12}$$

The ideal efficiency of a thermoelectric device for electricity generation, η_{max}, is given by [29,30]:

$$\eta_{\max} = \frac{T_H - T_L}{T_L}\cdot\left(1-\frac{1+\frac{T_L}{T_H}}{\sqrt{1+ZT}+\frac{T_L}{T_H}}\right) \tag{13}$$

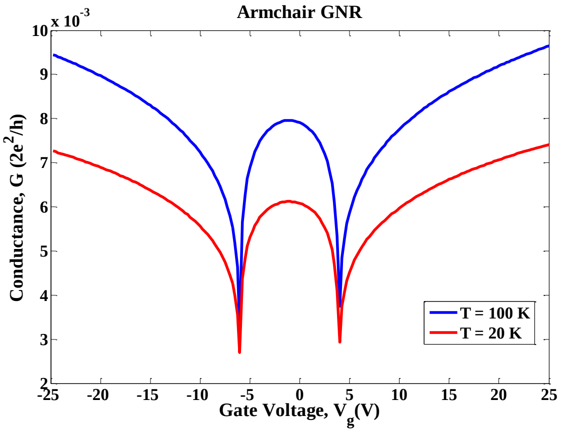
Where T_H is the temperature of the heat source (hot side of the present nanodevice) and T_L is the temperature of the heat sink or cold side of the present nanodevice. Eq.(13) relates the device efficiency to the figure of merit which a materials property and therefore most of the effort in the thermoelectric field is focused on materials development to improve the thermal to electrical conversion efficiency.

III. RESULTS AND DISCUSSION

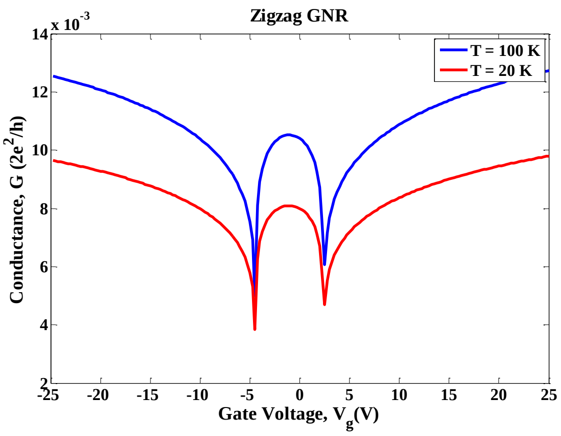
Numerical calculations are performed for the following thermoelectric parameters: Seebeck coefficient, S, (Eq.2), the electronic thermal conductance, κ_e, (Eq.3), the figure of merit, ZT, (Eq.11) and Nernst coefficient, N_T, (Eq.12). These thermoelectric parameters are for both strained armchair and zigzag graphene nanoribbons with certain widths. The present authors [24] investigated the quantum transport characteristics of both strained armchair and zigzag graphene nanoribbons field effect transistors. The band structure parameters of both graphene nanoribbons as the energy gap, the C-C bond length, the hopping integral, Fermi energy and the width are modulated by uniaxial tensile strain [24] (ε=15%). The value of the frequency, ω, of the induced ac-field equals 5×10^{12}Hz, and the value of applied magnetic field, B, equals 0.4 T.

The features of the results for the thermoelectric parameters and the electrical conductance for both armchair and zigzag graphene nanoribbons are:

-Figs. (1a,b) show the variation of the electrical conductance, G, with the gate voltage, V_g, for types of graphene nanoribbons at different temperatures T=20K, T=100K.



(a)

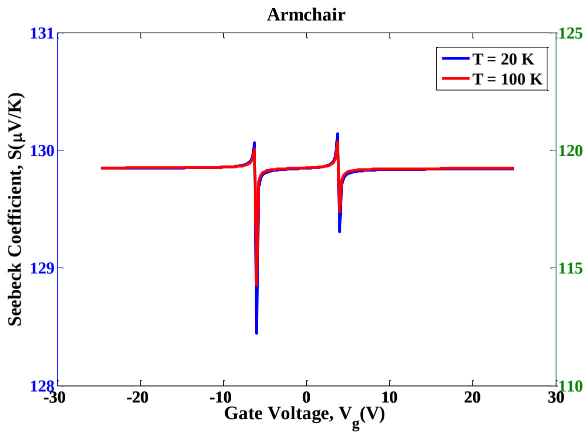


(b)

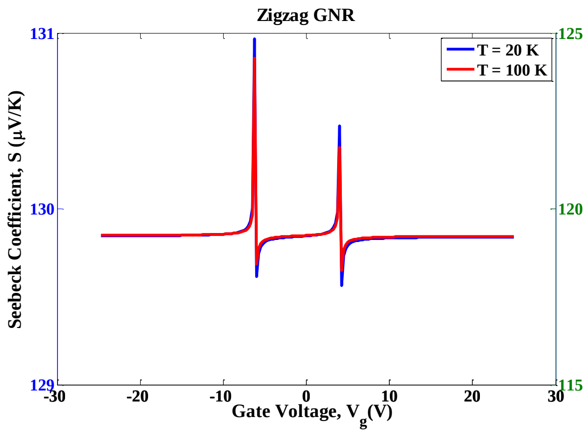
Fig.1. *The variation of conductance, G, with gate voltage at two different temperatures.*

As shown from Fig.(1a) that at T= 100, G_{min}= 0.0033 (V_g=-6V) & 0.0037 (V_g=4V) and at T=20K, G_{min}= 0.0027 (V_g=-6V) & 0.0029 (V_g=4V). While for Fig.(1b), we notice the following: at T= 100K, G_{min}=0.005(V_g = - 4.5V) & 0.0061(V_g =2.5V) and at T=20K, G_{min}=0.0038 (V_g=- 4.5V) & 0.0047 (V_g= 2.5V).

-Figs.(2a,b) show the variation of the Seebeck coefficient, S, with the gate voltage, V_g, at different temperatures T= 20K, 100K.



(a)

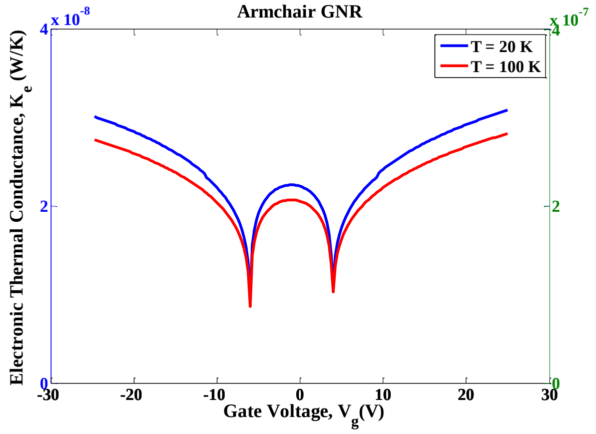


(b)

Fig.2. *The variation of Seebeck coefficient, S, with gate voltage at two different temperatures.*

As shown from Fig.(2a,b) that a resonant peaks and dips at certain gate voltage for the Seebeck coefficient for both armchair and zigzag graphene nanoribbons. We notice the peak heights for zigzag grapheme nanoribbon are greater than the peak heights for armchair graphene nanoribbon. This result shows that the values Seebeck coefficient for both armchair and zigzag graphene nanoribbons are enhanced strongly due to the induced uniaxial tensile strain [21-23, 27, 31].

-Figs.(3a,b) show the variation of the electronic thermal conductance, κ_e, , with the gate voltage at different temperatures T=20K, 100K.



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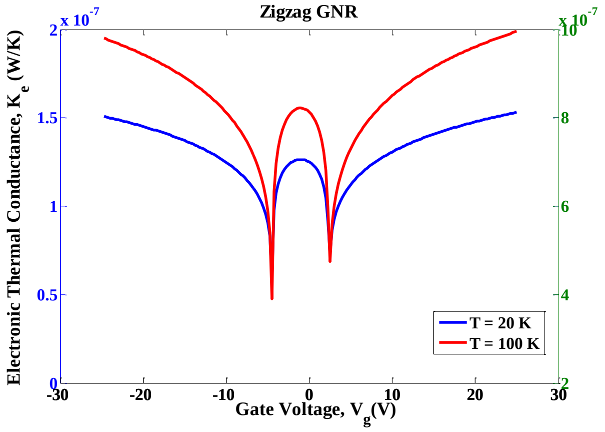
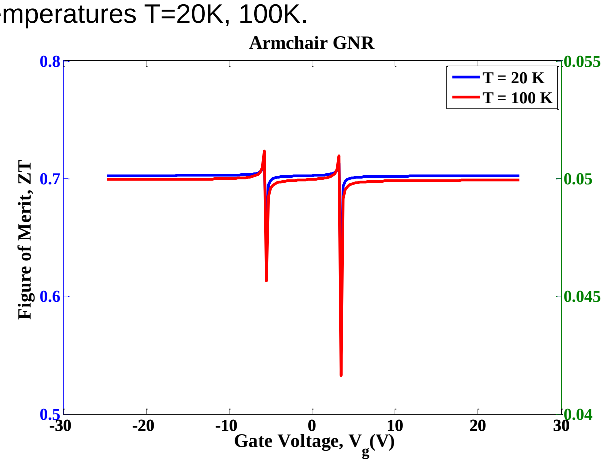


(b)

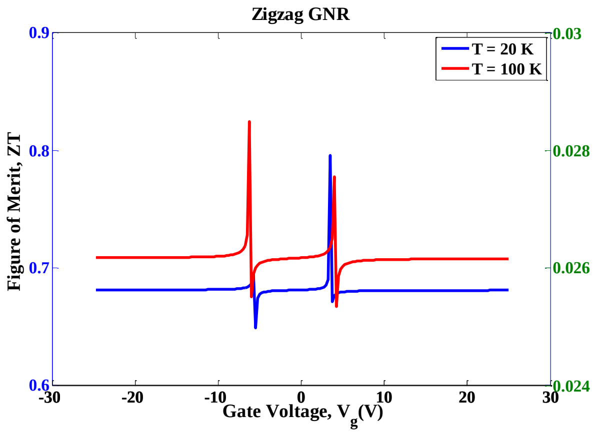
Fig.3. *The variation of electronic thermal conductance with gate voltage at different temperatures.*

We notice from Figs. (3a,b) that the trend of the electronic thermal conductance, κ_e,, is similar in a quit behavior of the electrical conductance, G,. This is expected result so as the electronic thermal conductance is related to the electrical conductance through Eq.(3). Also we notice from Fig.(3a,b) that the values of the electronic thermal conductance are small, this is expected result due the effect of the uniaxial tensile strain [2,21-23], which is needed for a good values of figure of merit, ZT, as will be shown below.

-Figs.(4a,b) show the variation of the figure of merit, ZT, with the gate voltage at different temperatures T=20K, 100K.



(a)



(b)

Fig.4. *The variation of the figure of merit with gate voltage at different temperatures.*

As shown from Fig.(4a), for armchair graphene nanoribbons that the maximum figure of merit are: $ZT_{max.}$= 0.7144 (V_g= -5.75V) at T=20K and at T=100K, $ZT_{max.}$=0.05116 (V_g=-5.75V). While for zigzag graphene nanoribbons, ZT_{max}=0.796 (V_g=3.5V) at T=20K and at T=100K, ZT_{max}=0.02849 (V_g=-6.25V). We notice from Figs.(4a,b) that figure of merit, *ZT*, exhibits peaks at the subband edges for both strained armchair and zigzag graphene nanoribbons [34]. Results show that the values of figure of merit, ZT, agree quietly well with those in the literatures [35, 36]. So, the present results for the figure of merit, ZT, might be predicted to be high enough to make them attractive for energy conversion.

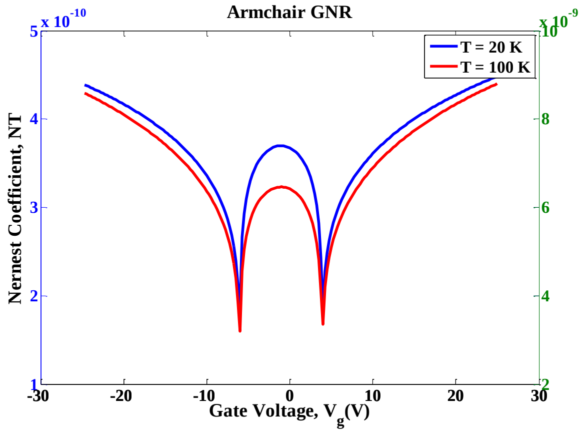
The table below shows the efficiency η of the present investigated thermoelectric nanodevice (Eq.(14)). From the table we notice that the efficiency, η, for zigzag graphene nanoribbon nanodevice is greater than those efficiency for armchair graphene nanoribbon nanodevice.

TABLE I. EFFICIENCY

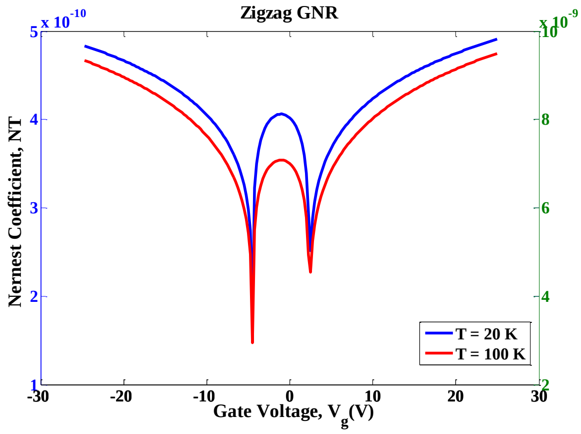
	Armchair	**Zigzag**
Efficiency (η) %	82	88.34

The present results show a high values of the efficiency, η, for the present investigated strained armchair and zigzag graphene nanoribbons. Since the efficiency of a thermoelectric nanodevice can be enhanced by increasing the power factor (S^2GT) or by decreasing the electronic thermal conductance. This has been achieved by applying tensile uniaxial strain to band structure of both types of graphene nanoribbons.

-Figs.(5a,b) show the variation of Nernst coefficient, N_T, with the gate voltage at different temperatures T=20K, 100K.



(a)



(b)

Fig.5. *The variation of Nernst coefficient with gate voltage at different temperatures*.

We notice from Figs.(5a,b) that the trend of Nernst coefficient for both armchair and zigzag graphene nanoribbons is similar to those of the electrical conductance (Figs.(1a,b)). Fig.(5a) shows two minima of Nernst coefficient for armchair graphene nanoribbons of 3.3573 x 10^{-9} at V_g = 4 V and 3.1944 x 10^{-9} at V_g = -6 V at (T=100 k) and two minima of Nernst coefficient of 1.8369 x 10^{-10} at V_g = 4 V and 1.8711 x 10^{-10} at V_g = -6 V at (T=20 k). While for Fig.(5b) shows two minima of Nernst coefficient for zigzag graphene nanoribbons of 4.5387 x 10^{-9} at V_g = 2.5 V and 2.951 x 10^{-9} at V_g = -4.5 V at (T=100 k) and two minima of Nernst coefficient of 2.5144 x 10^{-10} at V_g = 2.5 V and 1.7428 x 10^{-10} at V_g = -4.5 V at (T=20 k). From these figures we notice that the values for Nernst coefficient for both armchair and zigzag graphene nanoribbons increase when the temperature increases. The trend of Nernst coefficient, N_T, for both armchair and zigzag graphene nanoribbons are due to the effect of the tensile uniaxial strain which affect on the band structure, in general, [24]. The Nernst effect which is the transverse thermoelectric power (TEP) induced by a longitudinal thermal gradient in a perpendicular magnetic field [1,2,30]. Since the Nernst effect represents the entropy transported per unit charge carrier of Dirac fermions, then Nernst coefficient for both types of graphene nanoribbons increases with the increasing temperature (Figs.(5a,b) and are very sensitive to band structure of both graphene nanoribbons which is induced by the external tensile uniaxial strain [32, 33].

IV. Conclusion

The present paper investigated the thermoelectric effects in strained armchair and zigzag graphene nanoribbons nanodevice. From the obtained results, the electronic thermal conductance is reduced due to the induced strain. So accordingly, the figure of merit is enhanced and a high values of the thermoelectric efficiency.

Also according to the obtained results in the present paper, the Seebeck and Nernst effects might allowed us to understand better some specific features of the band structure under the effect of tensile strain and ambipolar quantum transport in one dimensional graphene nanoribbon. The results of the present research indicate that the strained graphene nanoribbon nanodevice might be promising for thermoelectric applications of energy conversion.

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