Carbon 126 (2018) 183–189

Contents lists available at ScienceDirect

Carbon

journal homepage: www.elsevier.com/locate/carbon

Influence of dephasing and B/N doping on valley Seebeck effect in zigzag graphene nanoribbons

Lei Zhang [a, b, e], Zhizhou Yu [c, b], Fuming Xu [d], Jian Wang [b, *]

[a] State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Laser Spectroscopy, Shanxi University, Taiyuan, 030006, China
[b] Department of Physics and the Center of Theoretical and Computational Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China
[c] School of Physics and Technology, Nanjing Normal University, Nanjing, 210023, China
[d] College of Physics and Energy, Shenzhen University, Shenzhen, 518060, China
[e] Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, 030006, China

ARTICLE INFO

Article history:
Received 13 July 2017
Received in revised form
29 September 2017
Accepted 6 October 2017
Available online 7 October 2017

ABSTRACT

We investigate the dephasing effect and atomic doping effect of random substitutional boron (B) or nitrogen (N) on the valley Seebeck effect in zigzag graphene nanoribbons (ZGNRs) using the tight-binding model calculations. When thermal gradient applied in the device made of ZGNRs is around several hundreds K, dephasing effect can only reduce the magnitude of pure valley current without generating electric current associated with the valley Seebeck effect. In the presence of B/N dopants, valley-polarized current occurs in ZGNRs. It is found that the generated valley polarized current is linearly dependent on the temperature gradient (ΔT) when the temperature of one lead is fixed and shows nonlinear dependence on temperature of a particular lead when ΔT is fixed. By calculating the phase diagrams such as $(\Delta T, p)$ with p the doping concentration, we find that the valley polarization can be tuned in a wide range from zero up to 0.72, indicating that it can be well controlled by B/N doping concentration. Finally, the noise power of valley Seebeck effect is also studied providing important information on the fluctuation of valley polarized current.

1. Introduction

In addition to charge and spin degrees of freedom, the manipulation and control of valley degrees of freedom of electrons attracted increasing attention in condensed matter physics community. In general, the valley index refers to the local maximum (minimum) of the valence (conduction) band in the first Brillouin zone [1–16]. As the potential information carrier, it can be utilized to store, manipulate and read out bits of information in the future electronics called valleytronics. Up to now, a variety of systems ranging from bulk to two dimensional materials have been proposed as potential building blocks of valleytronics, including silicon [1–3], bismuth [4], diamond [5], carbon nanotube [6], graphene [7–9,17], silicene [10], transition metal dichalcogenide monolayers (TMDs) [11–13,18–20], to just name a few. In particular, the successful isolation of 2D materials (such as graphene and TMDs) boost the rapid research advance in valleytronics. To achieve different functionalities in valleytronics, people proposed to use electric, magnetic, and optical means to manipulate and control the valley degree of freedom, which have been realized recently in experiment [11,18–20]. For instance, by applying the magnetic and optical field [11,20], the valley degeneracy in the system can be lifted and hence the valley polarized current can be generated and detected, which is extremely important for valleytronics.

Valleytronics may also find its application in caloritronics. Valley caloritronics [14–16], i.e., a combination of valleytronics and thermoelectrics, may provide an alternative way to harvest thermoelectric waste heat. Currently, the world energy consumption increases with an astonishing speed while huge amount of heat energy is wasted, which takes up a big portion in the energy loss. Therefore, the utilization of the heat waste becomes increasingly important. As a result, thermoelectricity has attracted great research attention in energy-saving technology [21,22]. Similar to spin caloritronics, the heat waste can also be used to induce the valley current in the absence of external bias voltage, which has great potential application in the future green energy technology. Indeed, the thermal means was recently proposed to generate the valley polarized current and as well as pure valley current without

* Corresponding author.
E-mail address: jianwang@hku.hk (J. Wang).

https://doi.org/10.1016/j.carbon.2017.10.017
0008-6223/

accompanying charge current [14–16]. As a result of a temperature gradient, the valley voltage difference across the system is generated which can drive the valley current in a valleytronic device. Since operation of valleytronic devices consume energy, in this sense, valley Seebeck effect can be used to harvest waste heat.

One of the important issues in valley caloritronics is to explore suitable materials for generation and manipulation of valley current using thermal means. In this work, we study the zigzag graphene nanoribbons (ZGNRs) for the following reasons. First of all, it has a very high melting temperature up to 4510 K and hence is thermally quite stable [23]. More importantly, two valleys in GNRs has a large separation in momentum space. The scattering due to the long wave length phonon between two valleys is small making the valley index a robust information carrier [8]. Note that our system involves temperature gradient so that the temperature in the central scattering region is not well defined at nanoscale. Since the temperature of leads are nonzero therefore there should exist phonons in the scattering region. However, since the temperature of the scattering region, where phonon is considered, is not well define, the relationship of the electron-phonon interaction and the temperatures of two leads will be very complicated. So rather than discussing this deep physics, we use a phenomenological theory in this paper, i.e., a dephasing mechanism to simulate the phonon, and use a parameter Γ_d to characterize the dephasing strength. In mesoscopic physics, it is known that the dephasing effect can have a large influence on quantum transport. For instance, dephasing effect can reduce the conductance when electron energy is near the resonance whereas an enhancement is observed in the case of off-resonance. It would be interesting to see what is the effect of dephasing on the valley current driven by thermal gradient. Furthermore, atomic doping in ZGNRs may provide another efficient way to tailor the electric transport properties of ZGNRs [24–30]. Therefore, it would be important to know whether doping effect can be used to modulate the valley Seebeck effect of ZGNRs and achieve different functionalities in valley caloritronics.

In this paper, we investigate the dephasing effect [31,32] and boron (B)/nitrogen (N) random atomic doping effect in the valley Seebeck effect of ZGNRs. It is found that by applying the temperature gradient across the device, the valley polarized current can be generated in the presence of B/N atomic doping. Furthermore, we find that the valley polarized current is linear with thermal gradient when the temperature of the right lead is fixed at 300 K. By increasing the doping concentration, the valley polarized current is decreasing while the electric current is increasing. Interestingly, the valley polarization can be effectively tuned by the doping concentration. This indicates that the doping mechanism can be used as an efficient tool in the application of ZGNRs in valley caloritronics.

2. Model and methods

In Fig. 1, a two terminal ZGNRs device with substitutional boron or nitrogen atomic dopants is shown. Here, B/N atomic dopants are randomly distributed in ZGNRs. In the tight-binding approximation of π orbitals, the Hamiltonian of ZGNRs can be expressed as

$$H = -t\sum_{\langle i,j\rangle}\left(c_i^\dagger c_j + c.c.\right) + \sum_{i\in d} V_i c_i^\dagger c_i, \tag{1}$$

where $c_i^\dagger$ (c_i) creates (annihilates) an electron on site i of ZGNRs. The first term of Eq. (1) represents the ideal ZGNRs with the nearest neighbor hopping energy t being 2.7 eV [33]. The second term of Eq. (1) describes the substitutional dopant with potential $V_i = 1.4$ or -1.4 eV for boron and nitrogen dopant located at site d, respectively [29]. In this study, we fix the size of ZGNRs device as $28.4\text{nm} \times 99.7\text{nm}$ and denote the doping concentration of B/N as p. Here we focus our attention to the zigzag graphene nanoribbon where the valley indices K and K' are well separated and well defined. While in the armchair graphene nanoribbon, K and K' points are mixed and hence is difficult to define two distinct valley indices. For the chiral nanoribbon, the distance between K and K is shorter than that in zigzag case. Therefore, the generation of valley polarized current due to the presence of B or N dopants should be larger than the case of zigzag for the same doping concentration.

In the framework of Landauer-Büttiker formula, the valley dependent current $I_{\alpha,\tau=K/K'}$ of αth lead driven by the temperature gradient $\Delta T = T_R - T_L$ can be written as

$$I_{\alpha,\tau} = \int \frac{dE}{2\pi}\sum_\beta\Big(f_\alpha(E) - f_\beta(E)\Big)\sum_{k\in\tau}\mathrm{Tr}\Big[\widehat{T}^k_{\alpha\beta}(E)\Big], \tag{2}$$

where $f_\alpha(E) = 1/(\exp[(E-E_F)/k_BT_\alpha]+1)$ denotes the Fermi-Dirac distribution of αth lead; E_F is the Fermi energy and T_α is the temperature in αth lead. In principle, the valley-resolved transmission operator $\widehat{T}^k_{\alpha\beta}(E)$ is defined as,

$$\widehat{T}^k_{\alpha\beta}(E) = \Gamma^k_\alpha G^r \Gamma_\beta G^a, \tag{3}$$

where $G^r = [G^a]^\dagger = [E - H - \sum_{\alpha=L,R}\Sigma^r_\alpha]^{-1}$ is the retarded and advanced Green's function, respectively. Here $\Gamma^k_\alpha = |W^k_\alpha\rangle\langle W^k_\alpha|$ is the linewidth function of αth lead with valley index τ and $|W^k_\alpha\rangle$ is eigenstate of $\Gamma_\alpha = i(\Sigma^r_\alpha - \Sigma^a_\alpha)$ with explicit momentum k [34–36]. Note that the traditional transmission coefficient $T_{\alpha\beta} = \sum_\tau\sum_{k\in\tau}\mathrm{Tr}[\widehat{T}^k_{\alpha\beta}(E)]$.

Therefore, the total valley and charge current $I_{\alpha,v/c}$ can be calculated by

$$\begin{aligned} I_{\alpha,v} &= I_{\alpha,K} - I_{\alpha,K'}, \\ I_{\alpha,c} &= I_{\alpha,K} + I_{\alpha,K'}. \end{aligned} \tag{4}$$

To examine the valley current and its correlation, we note from the bandstructure of ZGNRs shown in Fig. 1(b) that the right moving electron is locked with valley K while the left moving electron is locked with valley K' in the first subband of ZGNRs. To characterize the valley polarization of current induced by the first subband, we introduce the following quantity

$$\eta = \frac{|I_{L,K}| - |I_{L,K'}|}{|I_{L,K}| + |I_{L,K'}|} = \frac{I_{L,c}}{I_{L,v}}. \tag{5}$$

Due to the discrete nature of quantum transport process, the electron transport is stochastic and hence the current usually fluctuates [37]. In order to obtain additional information about the fluctuations of valley current, it will be very interesting to study the noise power of valley resolved current [38].

$$S_\tau = \int\frac{dE}{2\pi}\sum_{k\in\tau}\mathrm{Tr}\left\{[(1-f_L)f_L + (1-f_R)f_R]\widehat{T}^k_{LR} + (f_L - f_R)^2\widehat{T}^k_{LR}\left(I - \widehat{T}^k_{LR}\right)\right\}, \tag{6}$$

and hence the noise power of total electric current.

In order to simulate the dephasing effect of e-ph, we adopt the Büttiker approach [31], which the fictitious voltage probes are introduced into the system to mimic the influence of phase-relaxing scattering. The Büttiker approach can be modeled by a self-energy term Σ^r_d [31,39–41].