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Phonon Drag Thermopower in Silicene in Equipartition Regime at Room Temperature

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Abstract: ***Similar to graphene, zero band gap limits the application of Silicene in nanoelectronics despite of its high carrier mobility. In this article we calculate the contribution of electron-phonon interaction to thermoelectric effects in silicene. One considers the case of free standing silicene taking into account interaction with intrinsic acoustic phonons. The temperature considered here is at room temperature. We noticed that the contribution to thermoelectromotive force due to electron drag by phonons is determined by the Fermi energy. The explicit temperature dependence of the contribution to thermoelectromotive force deriving from by phonons is weak in contrast to that due to diffusion, which is directly proportional to temperature. Thus a theoretical limit has been established for a possible increase of the thermoelectromotive force through electron drag by the intrinsic phonons of silicene.***

Keywords: Phonon-drag thermopower, electron-diffusion thermopower, silicene, fermi energy, zero band gap

I. INTRODUCTION

Graphene and its nanoribbons belong to planar one-dimmensional (1D) and two-dimensional (2D) materials have accelerated the quick growth of nanoscience and nanotechnology. Silicene, a silicon analogue of graphene has the great advantage of its compatibility with the present industrial processes based on silicon nanotechnology. The most significant issue of silicene is instability in the air due to the nonplanar buckled structure. Silicene is expected to have a dirac-cone shaped energy band [1] and ultra-high carrier mobility [2] and thus has a potential application in high performance nanoelectronics. Recently, Silicene has been successfully grown on Ag [3-7], ZrB_2 [8], Ir [9] and MoS_2 [10] substrates. However, zero band gap of silicene limits its application as a logic element in electronic devices directly. It is very important to adjust the band gap of silicene without mortifying its carrier mobility. Silicene, which consists of Si atoms has a single layer of hexagonal honeycomb structure [6, 11-12]. Unlike graphene, the bonds between Si atoms are sp^2-sp^3 hybridization and the atoms are puckered rather than perfectly aligned in a single plane [13]. The properties of silicene can be easily tuned by an electric field due to its buckled structure. Therefore, silicene has extra potential to be applied in the electronic device industry. Considering the great properties of the graphene, the new structures such as 2D nanostructures from group IV of periodic table including silicene [6], germanene [14-15] have been considered. Some reports were published in early 2000 on the production of single layered nanosheet made by Si atoms, which is called Silicene [16]. It was shown that, the silicene is the thinnest possible silicon layer which possesses great physical properties [14] and has variety of applications [17].

It is very important to realize the transport properties of electronic materials from the point of view of emerging its physical concept and applications. There exists in literature, work discussing the study of transport properties of honey comb structured materials such as graphene [18] and silicene [19]. Shakouri et al [20] investigated the electronic charge transport through a zigzag silicene nanoribbon subjected to an external electric field. Lu et al [21] investigated the valley-dependent energy band as well as charge transport property of silicene nanosheet under a periodic potential. Theoretical investigation of thermopower of silicene in an external electric field perpendicular to silicene sheet has been studied and measured the thermopower of silicene is of the order of -80μV/K in the absence of electric field and it can be enhanced by several times when an electric field is applied externally [22]. Thermoelectric properties significantly depend on the electronic band structure and are enhanced when the fermi level is in the energy gap. Also thermoelectric efficiency is significantly reduced when the phonon contribution to the heat conductance is included which is calculated numerically by two different methods [23]. A study has been made which gives rise to a spin thermopower in addition to conventional Seebeck coefficient because coulomb interaction significantly modifies topological properties of a materials and thus also their transport and thermoelectric properties [24]. Thermoelectric figure of merit (FOM) upto 160 are achieved in silicene provided the fermi energy is located approximately 100 meV [25]. Zberecki et al [26] shown spin thermopower in silicene can be considerably enhanced by the impurity atoms. The mobility of carriers are calculated as a function of temperature and compared with the experimental results [27].

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Transport properties such as hot electron energy relaxation and thermopower at low temperature depend purely on electron-phonon interaction and are used as tools to determine the electron-phonon coupling strength. [28, 29]

The thermoelectric properties of any new materials can be realized by studying with its possible applications in thermoelectric devices as their efficiency depends upon the thermoelectric figure of merit Z. Phonon-drag thermopower S^g as well diffusion thermopower S^d is an important contribution to the total thermopower $S = S^g + S^d$, particularly at low temperature and it has been studied theoretically and experimentally in semiconductor heterojunction [30]. Theoretically S^g is studied in graphene [31], 3D Dirac and Weyl semimetals [32]. Diffusion thermopower is predicted to show linear temperature dependence for $k_B T \ll E_F$ (fermi energy, E_F ~200 meV) agreeing with Mott formula and experimental results [33]. The measured value of S^d at room temperature is about 62 μV/K.

In this present work, a theory of phonon-drag thermopower S^g in silicene is developed and studied numerically as a function of fermi energy at room temperature. The calculated value of S^g is enhanced to ~57 μV/K at fermi energy of 200 meV.

II. THEORY

It is assumed that the temperature is high enough to maintain an equipartition regime of electron-phonon interaction, in which the number of occupation of the acoustic phonon modes contributing to the phonon-drag effect are larger than 1. The phonons interacting with electrons have a wave vector on the order of k_F and energy $\hbar v_s k_F$. The Fermi energy is known to be related with carrier concentration n_s as $E_F = \hbar v_F \sqrt{\pi n_s}$ [34].

The kinetic equation for the equilibrium distribution function of phonon mode occupation numbers in the presence of temperature gradient is

$$v_s \frac{\boldsymbol{q}}{q} \frac{dN_{ph}^{(0)}(\boldsymbol{q})}{dT} k_B \nabla T = -\frac{N_{ph}^{(1)}(\boldsymbol{q})}{\tau_{ph}(\boldsymbol{q})} \tag{1}$$

where $\tau_{ph}(\boldsymbol{q})$ is the relaxation time of phonon with wave vector $\boldsymbol{q}$. Here, the relaxation time should be taken for the in-plane acoustic phonons with a wave vector magnitude from 0 to $2k_F$. The relaxation time of phonons in general generates the drag effect cannot be straightly connected with thermal conductivity of the sample because the phonons from whole Brillouin zone, the phonons from other branches and other mechanisms of phonon scattering including three-phonon normal and Unklapp processes at the temperature higher than 300K define total thermal conductivity of the sample.

According to Fermi golden rule, the rate of electron transitions from a state with wave vector $\boldsymbol{k}$ to a state with a wave vector $\boldsymbol{k'} = \boldsymbol{k} + \boldsymbol{q}$ driven by scattering from a phonon with wave vector $\boldsymbol{q}$ (involving absorption or emission of one acoustic phonon) is given by

$$W_{\boldsymbol{k}\to\boldsymbol{k}+\boldsymbol{q}}^{em,ab} = \frac{2\pi}{\hbar} \frac{N_{ph}(\boldsymbol{q})}{v_F \omega_{ph}(\boldsymbol{q})} \left|M_{e-ph}(\boldsymbol{q})\right|^2 \frac{A}{N_u M} \delta\left(k' - k + \frac{\omega_{ph}(q)}{v_F}\right) \tag{2}$$

where $\left|M_{e-ph}(\boldsymbol{q})\right|$ is the matrix element of electron scattering from a phonon specifying the magnitude of electron-phonon interaction, M is atomic mass of silicene, A is the sample area and N_u is the number of elementary cells in the sample. The combination of the three last quantities can be expressed through the surface density of silicene ρ = 7.2x10^{-8} gms/cm^{-2} and lattice constant a_0 =3.87A^0.

The matrix element depends on the phonon wave vector and the scattering angle $\theta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}}$ as $\left|M_{e-ph}(\boldsymbol{q})\right| = \frac{Dq}{2}\left(1 + \cos(\theta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}})\right)$ [ref] for long wavelength acoustic phonons. In case of completely isotropic electron scattering, $\left|M_{e-ph}(\boldsymbol{q})\right| = Dq$, the phonon drag thermopower would increase by fourfold. The quantity D is called acoustic deformation potential constant. Note that this value is very close to combination of $\left(\frac{2\pi\hbar v_F}{a_0}\right)$, which permits the estimation of silicene electron bands.

In the first order of perturbation theory the contribution to the drag comes from four different types of electron transitions, which correspond to the coming and leaving of electrons into the state with wave vector $\boldsymbol{k}$ following absorption and emission of a phonon with wave vector $\boldsymbol{q}$. The rate of variation of the electron distribution function mediated by interaction with phonons can be represented in the following equation in full form in the standard way through the phonon collision integral

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$$\left(\frac{d\,f(k)}{dt}\right)_{ph} = -\int \frac{dq}{4\pi^2}\Big[W^{ab}_{\boldsymbol{k}\to\boldsymbol{k+q}}\, f^{(0)}(\varepsilon_{\boldsymbol{k}})\left(1-f^{(0)}(\varepsilon_{\boldsymbol{k+q}})\right) + W^{em}_{\boldsymbol{k}\to\boldsymbol{k-q}}\, f^{(0)}(\varepsilon_{\boldsymbol{k}})\left(1-f^{(0)}(\varepsilon_{\boldsymbol{k-q}})\right) - W^{ab}_{\boldsymbol{k-q}\to\boldsymbol{k}}\, f^{(0)}(\varepsilon_{\boldsymbol{k-q}})\left(1-f^{(0)}(\varepsilon_{\boldsymbol{k}})\right) - W^{em}_{\boldsymbol{k+q}\to\boldsymbol{k}}\, f^{(0)}(\varepsilon_{\boldsymbol{k+q}})\left(1-f^{(0)}(\varepsilon_{\boldsymbol{k}})\right)\Big] \quad (3)$$

In equation (3), $f^{(0)}(\varepsilon_{\boldsymbol{k}})$ is the equilibrium distribution function of electrons with a chemical potential depending on ε_F and temperature. At low temperatures, the chemical potential can be assumed equal to $E_{\boldsymbol{F}}$ and the correction accounting for temperature variation may be neglected. The energy conservation law is fundamentally important including into equation (3) the distribution function of electrons before and after their scattering from a phonon [35]. One can take

$$f^{(0)}(\boldsymbol{k}+\boldsymbol{q}) = f^{(0)}(\boldsymbol{k}) \pm \frac{df^{(0)}(\varepsilon)}{d\varepsilon}\hbar\omega_{ph}(\boldsymbol{q}) \quad (4)$$

The positive sign indicates for absorption of a quantum of sound and negative sign for emission. Conversely, integrating in angle, we get

$$\delta\left(k' - k \pm \frac{\omega_{ph}(\boldsymbol{q})}{v_F}\right) \cong \frac{1}{q}\,\delta\left(cos\theta_{\boldsymbol{k.q}} + \frac{q}{2k}\right) \quad (5)$$

which corresponds to neglecting phonon energy in considering of scattering. As a result, interaction with a phonon flux transforms the collision integral to

$$\left(\frac{d\,f(\boldsymbol{k})}{dt}\right)_{ph} = v_F\frac{\boldsymbol{k}}{k}k_B\nabla T\, G_{ph}(k)\frac{df^{(0)}}{d\varepsilon} \quad (6)$$

where dimensionless parameter is introduced given by

$$G_{ph}(k) = \frac{S}{2MN_u}\frac{D^2}{\hbar^3 v_F^4}\frac{L}{v_S}\varepsilon^2(k) \quad (7)$$

The phonon collision integral can be interpreted as a field term of the Boltzmann kinetic equation. This makes possible calculation of the non-equilibrium term $f^{(1)}(\boldsymbol{k})$ for the electron distribution function $f^{(0)}(\varepsilon_{\boldsymbol{k}})$ in the relaxation time approximation by straightforward multiplication of the right-hand part of relation (6) by the electron transport relaxation time $\tau(\varepsilon_{\boldsymbol{k}})$. The final expression for the contribution provided by the phonon-drag thermopower becomes

$$S^g_{ph} = \frac{\pi^4 k_B\hbar L}{2eMa_0^2 v_S}\left(\frac{Da_0}{\hbar v_F\pi}\right)^2\left(\frac{E_F a_0}{\hbar v_F\pi}\right)^2 \quad (8)$$

The most remarkable feature in the relation obtained is that it does not contain an explicit dependence of thermopower on temperature, which argues with [36]. The obtained relation correlates with the observation that only a directed phonon flux contributes to thermopower; the flux is proportional to temperature gradient and does not depend directly on the temperature itself.

The results of phonon drag thermopower obtained from equation (8) can be compared with well known formula of carrier diffusion thermopower given by

$$S^d = \frac{\pi^2}{3e}\frac{k_B^2 T}{E_F} \quad (9)$$

This expression for the diffusion thermopower factor in the thermopower in silicone correlates with Mott formula and coincides with that derived for different materials.

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III. RESULTS AND DISCUSSION

We theoretically studied the dependences of the contribution to thermopower due to electron drag by phonons and of the contribution to thermopower due to diffusion as a function of Fermi level, which were calculated using equations (8) and (9) respectively using the characteristic of silicene material parameters, atomic mass, M =4.6637x10^{-26} kg, deformation potential constant, D=3.2 eV, sound velocity,v_s = 6.3x10^4 cm/s, lattice constant, a_0=3.87 A^0, phonon mean free path, L=12µm, and Fermi velocity, v_F=5.8x10^7 cm/s.

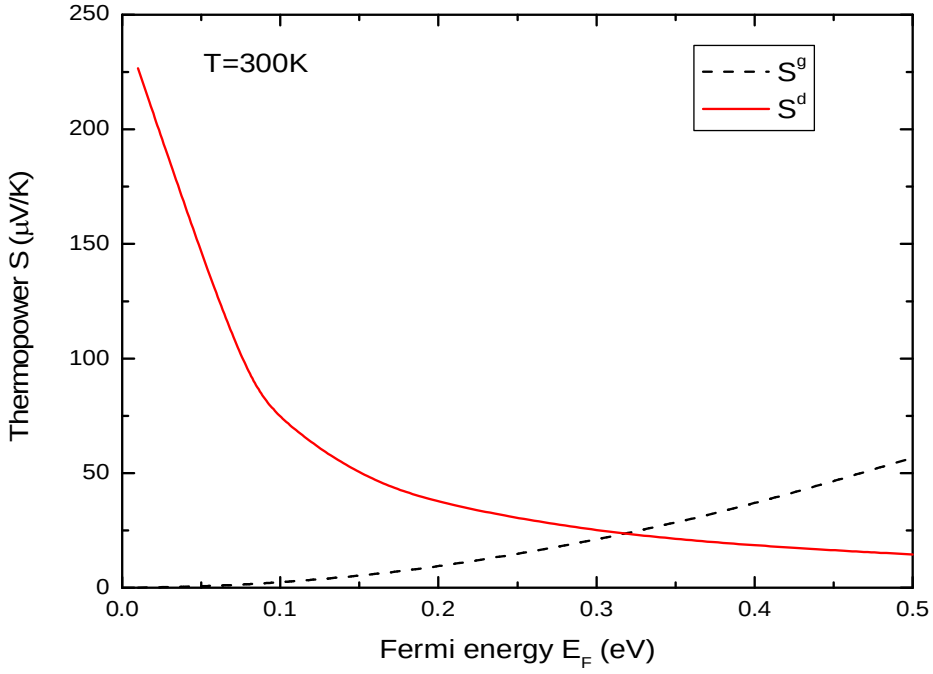


Figure 1: Graph of thermopower against Fermi energy at room temperature. Dashed black line represents the contribution from phonon drag effect and red line represents contribution from diffusion thermopower.

In most of the existing literature, straightforward calculations were made on thermopower interms of the Mott formula [37], showing no phonon drag contribution in these studies. Figure (1) shows the contribution from drag thermopower to total thermopower measured at fermi energy of about 200 meV at room temperature which can be compared with diffusion thermopower. We chosen Fermi energy as 200 meV because the diffusion thermopower shows linear dependence with temperature at 200 meV [33]. At low temperatures, Mott formula was existing with small deviations. These deviations should most likely be assigned only to a decline of measurement accuracy. Zuev et al [38] suggest enlargement of thermopower with increasing Fermi level. The first reason for the phonon drag effect becoming suppressed could be the reverse effect exerted by electrons on the phonon system, accompanied by the corresponding decrease of the phonon relaxation time [35]. The second possible factor could be the effect of the substrate, which may likewise reduce the phonon mean paths.

The phonons that generate the drag of electrons are very small part of the excited phonons that define thermal conductivity. In theory it allows to manipulate the thermal conductivity ad the phonon drag thermopower separately. We suggest that the phonon drag thermopower is defined by the scattering of phonons on the edges of the silicene sample. Thermal conductivity can also rise nearly up to the room temperature with increasing sample size. But due to relation $ZT = \frac{\sigma TS^2}{\kappa}$ (κ being the thermal conductivity) for the thermoelectric figure of merit, it will grow with increasing of sample size linearly or even faster. The problem of the thermal conductivity reducing is complicated because making samples with point defects, placing samples onto the substrate or increasing ambient temperature will reduce both electrical and thermal conductivity of the sample and these effects should be considered simultaneously. Therefore, tuning the size of the sample seems to be the straightest way of improving silicone thermoelectric properties.

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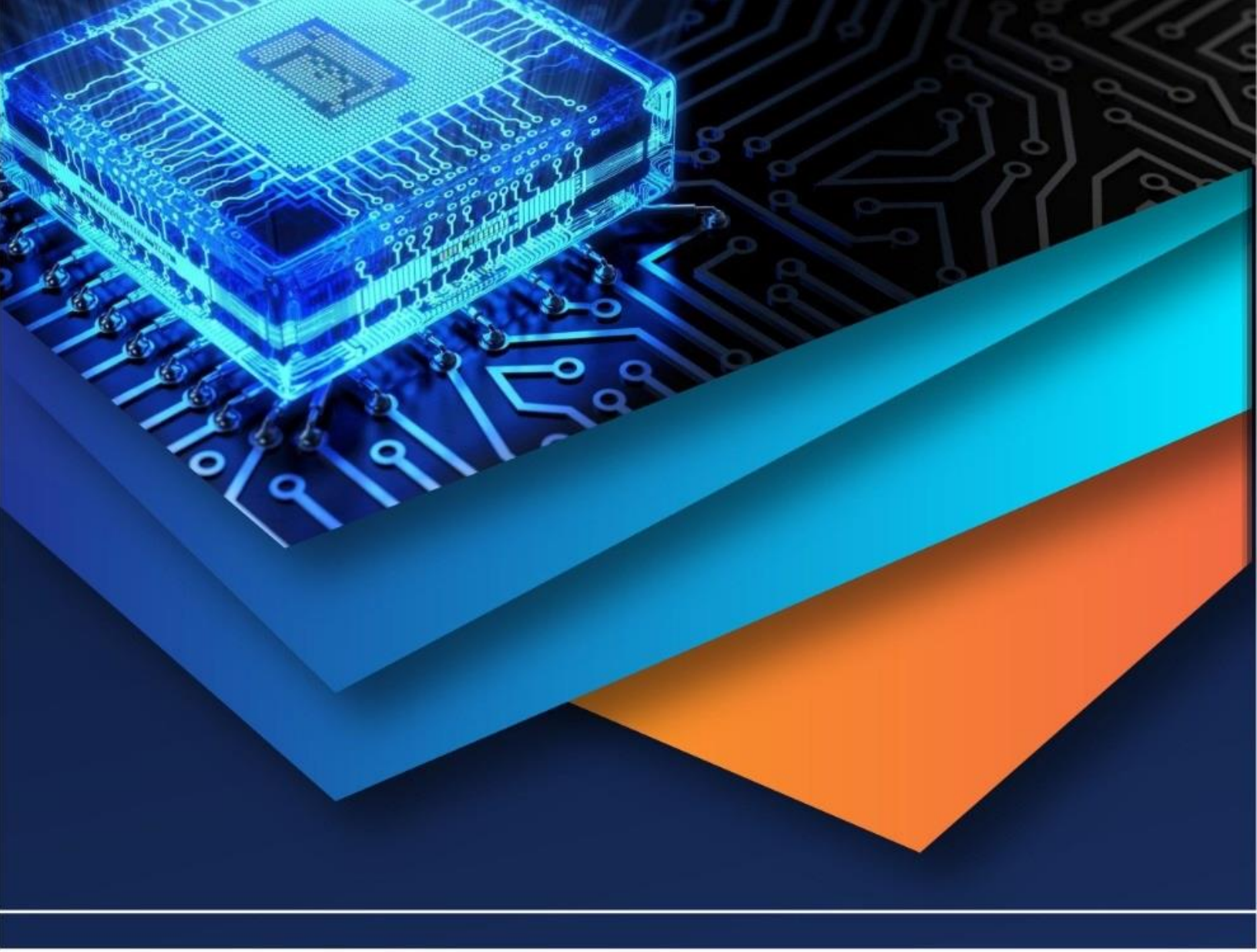
IV. CONCLUSION

In this study, we conclude that in a high quality sample with a large phonon mean free path, which probably correlates with high thermal conductivity at room temperatures and at a high Fermi level one may expect the contribution to thermopower due to phonon drag to dominate over the diffusion-associated one, and a sharp increase of the Seebeck coefficient and thermoelectric figure of merit.

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