

Study the properties of conductivity in two-layer graphene using mathematical modeling

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Abstract. Graphene is a two-dimensional allotropic form of carbon, with atoms combined into a hexagonal crystal lattice, forming a layer one atom thick. Graphene possessing exceptional optical, mechanical, physical and electrophysical properties. This article details some of the conductivity in graphene. The conductivity of the two-layer graphene was measured by special mathematical models, with conductivity dependent on the voltage at the gate at different temperatures. Conductivity is faced with a jump at zero temperature and a sharp, standard rise in properties at room temperature, as shown clearly in the resulting electronic spectrum.

1. Introduction

Graphene is a two-dimensional allotropic form of carbon, which is formed by a layer of carbon atoms one atom thick, located in sp^2 hybridization and connected via σ and π bonds to a two-dimensional hexagonal crystal lattice (Fig. 1). The distance between adjacent atoms of the crystal lattice is graphene is 0.142 nm. Graphene can be represented as one atomic plane of a natural carbon species - graphite, separated from a bulk crystal [1]

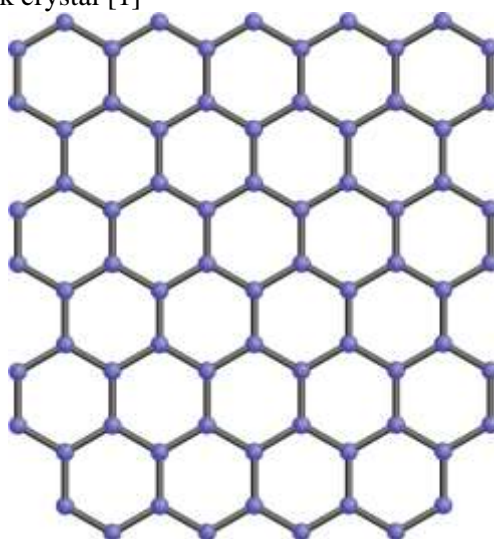


Figure 1. Structure diagram of the graphene crystal lattice.

For a long time, scientists could not get stable graphene samples. The atomic plane of graphene sought to minimize its surface energy and curled up, transformed into various allotropic forms of carbon - amorphous carbon, carbon nanotubes and fullerenes[2].

Only in 2004, a group of scientists from the University of Manchester and the Institute of Microelectronics Technology Problems in Chernogolovka under the guidance of Andre Geim and Konstantin Novoselov obtained graphene using ordinary tape and tape. The graphite synthesized by them was transferred onto a 300 nm thick silicon oxide substrate. Due to light interference, sections of different plate thicknesses had different colors[3]. The thinnest sections of this plate were almost colorless. Among them, using atomic force microscopy, the structure of one atomic plane of graphene was discovered[4].

The new carbon modification has unique properties. The mechanical strength of graphene is twice that of steel. The thermal conductivity of graphene is 10 times that of copper.

Graphene is characterized by a linear law of electron dispersion. Quanta of a light wave or electromagnetic radiation - photons, which are massless particles that propagate in space at the speed of light, have the same energy dependence on momentum. In graphene, electrons, like photons, have no mass. But their charge is not equal to zero and the speed of their movement is 300 times less than that of c

Due to the linear dispersion law, graphene is a semimetal, which is a semiconductor with zero band gap and conductivity not inferior to the conductivity of copper. The mobility of electron graphene is greater than that of all known materials (100 times greater than that of silicon).

Graphene also has unique optical properties[5]. The transmission coefficient of the light wave for graphene in the region of visible light is described by the formula:

$$T \approx 1 - \pi\alpha \approx 97,7 \%, \quad (1)$$

where α is the fine structure constant.

Thus, graphene absorbs only about 2.3% of the light waves of the visible radiation range. That is, graphene plates are almost transparent.

The transparency, good electrical conductivity and elasticity of graphene make it a promising material for the creation of solar cells and touch displays. In all respects, graphene is much better suited for such devices than the indium tin oxide currently used[6,7].

To calculate the electron current density in Graphene, we use an analog of the Landauer-Buttiker formula for the two-dimensional case, in other words, we calculate the difference in the fluxes of electrons moving from the source to the sink and back:

2. Calculation of conductivity and current density

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$$j = \frac{e}{\pi^2 \hbar^2} \int v_x D [f(\varepsilon(p), \mu) - f(\varepsilon(p), \mu - |e|V_D)] dp_x dp_y, \quad (2)$$

in which $f(\varepsilon(p), \mu)$ and $f(\varepsilon(p), \mu - |e|V_D)$ are the electron distribution functions at the source, respectively $v_x = d\varepsilon/dp_x$ is the group velocity of the electron, and the transparency coefficient of the barrier D depends from the energy and momentum of a flightless particle. In our model, we neglect the tunneling effect (the calculation of this phenomenon has already been done before us), therefore, the transmission coefficient can take values only 0 or 1, depending on the energy and momentum of the particle. We rewrite (2) in a more convenient form

$$j = \frac{e}{\pi^2 \hbar^2} \int D(\varepsilon, p_y) [f(\varepsilon, \mu) - f(\varepsilon, \mu - |e|V_D)] dp_\varepsilon dp_y, \quad (3)$$

If $|p_y| \leq p_{min}$, then the incident particle can be reflected from the barrier only if it reaches the minimum of the band structure, i.e. for $\varepsilon - e\phi \leq \varepsilon_{min}$. But this condition coincides with the requirement ($\varepsilon \leq \varepsilon_{min} + e\phi$), therefore, all particles with momenta $|p_y| \leq p_{min}$ are simultaneously included in the current transfer process if their energy $\varepsilon \geq \varepsilon_{min} + e\phi$.

If $|p_y| \geq p_{min}$, then the incident particle will no longer reach the minimum of the band structure, and therefore reflection will occur only if it loses its entire longitudinal momentum p_x . This will happen when $\varepsilon - e\phi = \varepsilon(p_x = 0, p_y)$, or, what is the same, when $|p_y| = p(\varepsilon - e\phi)$. Here $p(\varepsilon)$ is the function inverse to the energy spectrum (we mean the branch with $|p_y| \geq p_{min}$).

Summarizing the above reasoning, we can “cut off” the integration limits in the expression for the current ($\varepsilon \leq \varepsilon_{min} + e\phi$), leaving only those momenta and energies for which the transmission coefficient is unity:

$$j = \frac{|e|}{\pi^2 \hbar^2} \int_{\varepsilon_{min} + e\phi}^{\infty} d\varepsilon \int_{-p(\varepsilon - e\phi)}^{p(\varepsilon - e\phi)} dp_y [f(\varepsilon, \mu) - (f(\varepsilon, \mu) - |e|V_D)], \quad (4)$$

Or by integrating over the transverse momentum explicitly

$$j = \frac{2|e|}{\pi^2 \hbar^2} \int_{\varepsilon_{min} + e\phi}^{\infty} p(\varepsilon - |e|\phi) [f(\varepsilon, \mu) - f(\varepsilon, \mu) - |e|V_D] d\varepsilon \quad (5)$$

This is the final formula for calculating the current. Note that in all the above arguments, we secretly assumed that for electrons in the upper gate region a barrier of height $e\phi > 0$ was created. For $e\phi < 0$ in (4), energy integration should be carried out not from $\varepsilon_{min} + e\phi$, but from ε_{min} , in the integrand expression should be $p(\varepsilon)$.

In the case of $e\phi > 0$, in expression (5) it is convenient to make the change of variable $\tilde{\varepsilon} = \varepsilon - e\phi$, which can be interpreted as the transfer of the integration domain to the contacts[8]. The expression for the current takes the form:

$$j = \frac{2|e|}{\pi^2 \hbar^2} \int_{\varepsilon_{min}}^{\infty} p(\tilde{\varepsilon}) [f(\tilde{\varepsilon}, \mu - e\phi) - f(\tilde{\varepsilon}, \mu - e\phi - |e|V_D)] d\tilde{\varepsilon} \quad (6)$$

Now, calculating the response to an infinitesimal bias voltage dV_D is not difficult: assuming that the Fermi functions in the contacts are shifted on the energy scale by an infinitely small value $|e|dV_D$, we can expand

$$f(\tilde{\varepsilon}, \mu - e\phi) - f(\tilde{\varepsilon}, \mu - e\phi - |e|V_D) = \frac{\partial f}{\partial \varepsilon} |e|dV_D, \quad (7)$$

and at low temperatures $T \ll \mu$ we can assume that $\partial f / \partial \varepsilon = \delta(\tilde{\varepsilon} - (\mu - e\phi))$. This leads to the following expression for the conductance $G = dj/dV_D$ (we will also call this quantity conductivity, although it is measured in $(\text{Ом} \cdot \text{м})^{-1}$, this should not cause misunderstanding):

$$G = \frac{2e^2 P(\mu - e\phi)}{\pi^2 \hbar^2}. \quad (8)$$

Due to the fact that expression (8) contains the function $p(\mu - e\phi)$, defined only for $\varepsilon \geq \varepsilon_{min}$ and equal to P_{min} , the conductivity based on bilayer graphene must experience a jump equal to

$$\Delta G = \frac{e^2 g k_{min}}{\hbar \pi}. \quad (9)$$

This jump occurs when the bottom of the conduction band touches the Fermi level in the source contact, i.e. for $\mu = e\phi + \varepsilon_{min}$. For the band gap $\Delta = 0.2 \text{ эВ}$, the wave vector $k_{min} = 4 \text{ нм}^{-1}$, which corresponds to the jump in conductivity $\Delta G = 1.25 \cdot 10^4 (\text{Ом} \cdot \text{м})^{-1}$. The inverse resistance jump turns out to be $(GW)^{-1}$ (W is the width of the graphene tape) and can take any value, unlike one-dimensional systems, where it was equal to $2h/e^2$. In principle, formula (8) together with (9) can be used to analytically calculate the conductivity as a function of the gate voltage at zero temperature. This problem, however, reduces to solving an algebraic equation of the fourth degree; the results of the solution are not visual. At finite temperatures, a semi-analytical calculation of conductivity is possible[9].

We substitute the expansion for the current expression:

$$\varepsilon_b \frac{\phi - V_{BG}}{d_b} + \varepsilon_t \frac{\phi - V_{TG}}{d_t} 4\pi |e| \Sigma_e - \Sigma_h \quad (10)$$

integrate by parts and divide by voltage drop dV_{DS} :

$$G = \frac{\partial j}{\partial V_{DS}} = \frac{2e^2 g p_{min}}{(2\pi\hbar)^2} f_F(\varepsilon_{min}, \mu - e\phi) + \frac{2e^2 g}{(2\pi\hbar)^2} \int_{p_{min}}^{\infty} f_F(\varepsilon(p), \mu - e\phi) dp \quad (11)$$

The obtained expression consists of two parts - the first line corresponds to the isotropic shift of the spectrum of two-layer graphene and leads to the existence of a conductivity jump at zero temperature, it disappears at $p_{min} = 0$. The second term corresponds to the usual quadratic spectrum $\varepsilon(p) \sim p^2$. In the case of an arbitrary temperature, the Fermi distribution function in explicit form begins to enter the formulas for the concentration and current; moreover, we must take into account the contribution of holes to the total charge density[10,11].

In this case, for the charge density in the channel $n_{ch} = \Sigma_e - \Sigma_h$, we should write:

$$n_{ch}(e\phi) = \frac{2}{\pi\hbar^2} \int_{q_{min}}^{\infty} [f(\varepsilon(p), \mu - e\phi) - f(\varepsilon(p), -(\mu - |e|\phi))] p dp, \quad (12)$$

where the second term under the integral sign corresponds to the contribution of holes to the charge density.

The smooth channel equation in this case is modified:

$$\frac{\varepsilon_t}{4\pi d_t} (V_G - \varphi) = \frac{|e|}{2} [n_{ch}(e(\varphi + V_D)) + n_{ch}(e\varphi)] \quad (13)$$

It is now interesting to trace the evolution of conductivity and linear current density as a function of the gate voltage with changing temperature - in Fig. 2 and fig. Figure 3 shows graphs for three temperatures: helium $T = 4 K$, nitrogen $T = 77 K$, and room $T = 300 K$.

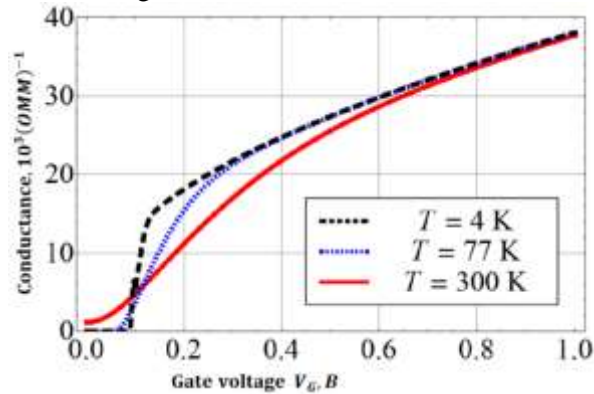


Figure 2. The dependence of the two-layer graphene conductivity on the cross-gate voltage at different temperatures.

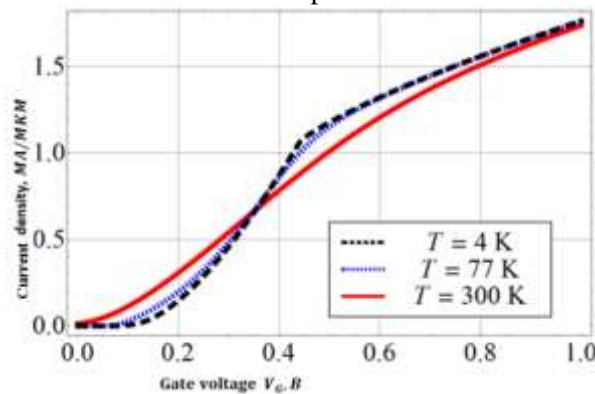


Figure 3. The dependence of the current density in two-layer graphene on gate voltage at different temperatures.

Analyzing the obtained curves, we see that the ratio of the currents on and off on two-layer graphene is of the order of 10 at room temperature and a gate voltage variation range 0.5 B V. That is why the methods for increasing the band gap in two-layer graphene attract considerable attention of researchers. we can say that the characteristic at room temperature inherits from the jump in conductivity at $T = 0$ a high slope. In the next subsection, we estimate this value analytically.

When the Fermi energy coincides with the temperature, it can be expressed in the following formula[11]:

$$|e|\Delta\varphi = T \quad (14)$$

If at zero temperature the jump in conductivity is equal to ΔG , then the derivative of conductivity at the point of the jump at a nonzero temperature can be estimated as

$$\frac{dG}{dV_V} = \frac{\Delta G}{\Delta d_G}$$

After this, the expression for the concentration of charge carriers takes the form

$$\Sigma_e(|e|\Delta\varphi, T) = \frac{2}{\pi\hbar^2 v^2} \int_{q_{min}}^{\infty} \left(1 + \exp\left\{\frac{(q-q_{min})^2}{2mv_F^2 T}\right\} - 1\right)^{-1} q dq, \quad (15)$$

The integral in (3.19) is taken analytically. After substituting its values in the formula for the connection of the potentials ΔV G and ϕ , we obtain

$$|e|\Delta V_G = T + \frac{8e^2 d_t}{\varepsilon_t \hbar^2} \cdot \left\{ \ln(1 + e) mT + 0.91 q_{min} \sqrt{\frac{2mT}{v_F^2}} \right\}, \quad (16)$$

0.91 is the approximate numerical value of the integral

$$\int_0^{\infty} \frac{dt}{1 + e^{t^2 - 1}}.$$

In short form, the voltage at the gate

$$\Delta V_G = aT + b\sqrt{T}, \quad (17)$$

where a and b are functions of both the spectrum of bilayer graphene and the structure parameters. For the above structural parameters (temperature is expressed in electron volts)

$$\Delta(|e|V_G) = 4.266T + 0.8775\sqrt{T}, \quad (18)$$

$$\frac{dG}{dV_V} = \frac{\Delta G(T=0)}{4.266T + 0.8775\sqrt{T}}, \quad (19)$$

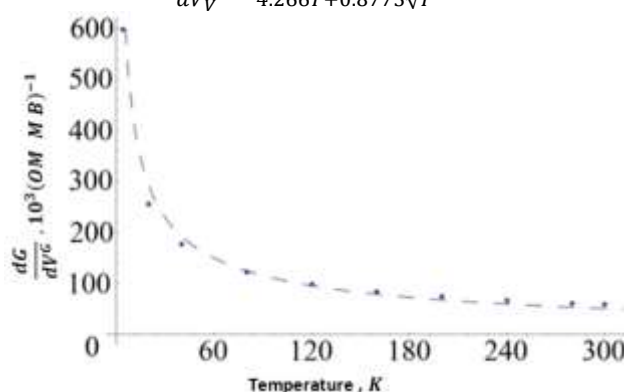


Figure 4. Comparison of the estimated maximum slope of the characteristic (dashed line) and the exact numerical calculation (points).

We note that the presence of a term proportional to \sqrt{T} in the denominator occurs again due to the presence of an isotropic shift along the momentum axis in the spectrum of bilayer graphene.

In fig. Figure 4 shows a comparison of the steepness calculated by the estimation formula (solid line) with the values obtained by an exact numerical calculation. The slope value for two-layer graphene with the indicated structure and spectrum parameters is $55 \cdot 10^3 \text{ (Ohm} \cdot \text{m} \cdot \text{V)}^{-1}$, which is an order of magnitude greater than the similar value for the type “silicon on the insulator” ($5 \cdot 10^3 \text{ (Ohm} \cdot \text{m} \cdot \text{V)}^{-1}$), which is considered as one of the most promising in silicon electronics[11,12,13].

3. Results

The aim of this work is to study the photon effect on graphene and carbon nanotubes.

In considering the photon effect on graphene and carbon nanotubes, the following conclusions were drawn:

- The high transmission coefficient of the light wave of graphene in combination with good electrical conductivity and elasticity make it a promising material for the creation of solar cells and touch displays.
- Only semiconductor modifications of graphene have optical properties.
- Graphene semiconductors are the best electronic emitters. The reason for this is its high electrical conductivity.
- Due to the sharp tip of graphene, high emission is possible even when low voltage is applied. The resulting emission current has a high density and extreme stability.
- Owing to their optical and semiconductor properties, subminiature size, good electrical conductivity, high emission characteristics and the ability to attach chemical graphene radicals, they have a wide range of applications in optoelectronics, measurement technology, chemical technology and biomedicine. Therefore, further detailed study of the properties of graphene is necessary.

- The problem of developing economical technologies for the mass production of graphene having predetermined properties and controlled sizes is one of the most important tasks of modern science.

4. Conclusion

To determine the promising capabilities of graphene-based devices, mathematical models are widely used due to technological adherence to the manufacture of real samples. The graphene conductivity model is explained by the graphene resistance depending on the voltage at the control electrode. It turns out that the maximum resistance resulting from the spread of a strong electron hole depends poorly on temperature. The characteristics of the resulting electronic spectrum show that the conductivity at zero temperature faces a jump, and this indicates the sharp and standard height of the properties at room temperature.

Dual-wall graphene is used because of its rigidity and flexibility and is useful for devices that depend on the effect of photons on the graphene because the photon is emitted under the influence of the electric field by high magnetic fields.

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