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The Electron Density of States in Graphene on a Substrate with a Local Structural Disorder

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In this paper we have obtained expression for the contribution to DOS with the help of the method of the temperature Green functions. Multiple elastic electron scattering by impurities and structural inhomogeneities in graphene on a substrate, has been taken into account. The resulting expression for the contribution to DOS depends on temperature, concentration of impurities and the type of short-range order (structural heterogeneity).

Keywords: Graphene, Density of Electron States, Structural Inhomogeneities.

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1. INTRODUCTION

The study of the electron density of states (DOS) in graphene is necessary to understand the processes of electron transport in these materials. DOS in graphene can be influenced by various factors such as temperature, concentration of impurities, structural defects, etc. Experimental and theoretical studies show that at low temperatures DOS in pure graphene is linearly dependent on energy [1]. It is also noted that adsorption of hydrogen by graphene opens the gap in DOS and, as a result, graphene becomes a semiconductor [1]. However the disordering of graphene structure (without adding of impurities) leads to its metallization [2].

In this paper we have obtained expression for the contribution to DOS with the help of the method of the temperature Green functions. Multiple elastic electron scattering by impurities and structural inhomogeneities in graphene on a substrate, has been taken into account.

2. CALCULATIONS

2.1 Relaxation time

The low-temperature peculiarities of DOS in graphene on a substrate may be described in the frame of the temperature Green functions (GFs) method [3, 4]. We have calculated inverse relaxation time $\frac{1}{\tau} = -\operatorname{Im}\Sigma$ and contribution to DOS $\Delta\nu = -\frac{1}{\pi}\operatorname{Im} Sp(\langle G\rangle - G_0)$. Here - Σ is self-energy part calculated taking into account multiple elastic scattering of electrons on structural inhomogeneities which are formed in the graphene plane on a substrate and described by short-range order parameters α_i [5]. $G_0 = \left(\varepsilon - \varepsilon_p + i0\right)^{-1}$ is the electron Green function in a perfect graphene, $\langle G\rangle$ is the averaged Green function in a disordered graphene and, finely, $\varepsilon_p = \hbar k \upsilon_F$ is the electronic spectrum in the ideal graphene plane near ε_F, where the Fermi velocity is $\upsilon_F \approx 10^6 m/s$ [6].

The obtained expression for the relaxation time is the following:

$$\frac{1}{2\tau} = \frac{1}{2\tau_{imp}}\left(1 + \sum_{i=0}^{N}\alpha_i B T^{-1/2}\right),$$

here $\sum\alpha_i$ are the short-range order parameters, N is the number of atoms in the range of structural inhomogeneity, $B = \frac{2\sqrt{2\pi}(1-c)}{\nu_0 N} m^{3/2} \approx 1.4K^{-1/2}$, $\nu_0 \approx \frac{p_0 m}{2\pi^2}$, c is the concentration of impurities, p_0 is the Fermi momentum, N - number of atoms in the range of structural inhomogeneities and m is electron mass. The inverse relaxation time of electron scattered only by impurities $\frac{1}{\tau_{imp}}$ is in order of $10^{14} s^{-1}$.

2.2 DOS

The contribution to DOS in graphene is defined as follows

$$\Delta\nu = -\frac{1}{\pi}\operatorname{Im} Sp(\langle G\rangle - G_0).$$

The resulting expression of contribution to DOS in disordered graphene consists of two terms:

$$\Delta\nu = \frac{1}{\hbar^2\upsilon_F^2}\left[\frac{\hbar}{2\tau}\ln\left(1 + \frac{p_0\upsilon_F(p_0\upsilon_F - 2\varepsilon))}{\varepsilon^2 + \left(\hbar/2\tau\right)^2}\right) + 2\varepsilon\, arctg\left(\frac{p_0\upsilon_F\left(\hbar/2\tau\right)}{\left(\hbar/2\tau\right)^2 + \left(\varepsilon - p_0\upsilon_F\right)\varepsilon}\right)\right].$$

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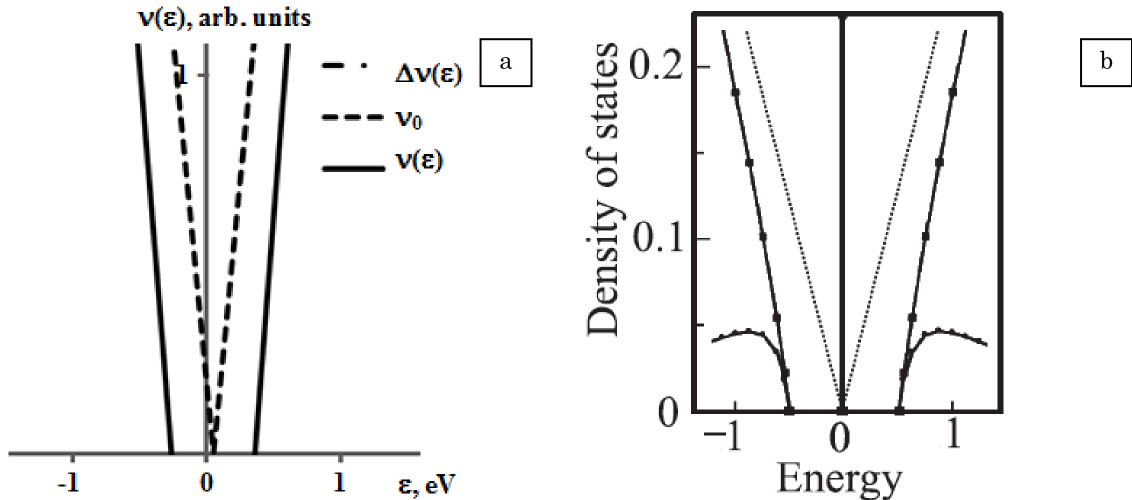

Fig. 1 – The calculated contribution to DOS obtained at *T=30K* for ∑α=-0.2 (dash-dot line), DOS for pure graphene $\nu_0(\varepsilon)$ (dotted line) and full DOS $\nu(\varepsilon) = \nu_0 + \Delta\nu$ (full line) (a) ; DOS calculated using the simplified M-model for pure graphene (dotted line) and for graphene saturated by hydrogen (full line) [3] (b)

3. RESULTS

The resulting expressions for the contribution to DOS depend on concentration of impurities and the parameters of short-range order (structural heterogeneity). Analyzing these expressions we concluded the following:

1. Gas adsorption in graphene leads to appearance of a gap in the DOS at the Fermi level, which can be explained by the negative contribution to DOS from multiple elastic electron scattering by structural inhomogeneities of short-range order (Fig. 1).

2. Change in the defect structure of graphene results in metallization of disordered graphene due to the increasing contribution to DOS at the Fermi level from the electron scattering by structural inhomogeneities of short-range order. This result is in a good agreement with data [2].

3. The value of $\Delta\nu(\varepsilon_F)$ increases when temperature rises in graphene without impurities (the case of metallization) and decreases in graphene saturated gas [6].

4. DISCUSSION

The results of our calculations showed that the low-temperature behavior of DOS is determined by the short range ordered structure of non-ideal graphene. At the same time the change in concentration of impurities does not strongly influence on the low-temperature DOS.

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