Indirect interaction of the carbon atoms as the origin of the epitaxial graphene frequencies shift

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To determine the effect of the substrate on the optical frequency $\omega_{LO}(\Gamma)$ of free-standing graphene, the problem of the adsorbed on a solid substrate dimer, consisting of two carbon atoms bound by direct (kinetic) t and indirect t_{ind} (through the state of the substrate) exchanges, is considered. It is shown that in the case of a semiconductor substrate, the resulting interaction is $t + |t_{ind}|$, which leads to a frequency $\omega_{LO}(\Gamma)$ shift by $\Delta\omega_{LO}(\Gamma) > 0$ (red shift of the Raman G-peak) and a relative shift $\delta_{LO}(\Gamma) \equiv \Delta\omega_{LO}(\Gamma)/\omega_{LO}(\Gamma) \approx |t_{ind}|/t$. The numerical estimates of $\delta_{LO}(\Gamma)$ made for the $6H$-SiC substrate are in good agreement with the experimental data. In the case of a transition metal substrate, it is shown that for metals with large effective masses of d-electrons (elements of the end of the $3d$-series), a situation $\Delta_{LO}(\Gamma) < 0$ is possible (blue shift), which actually takes place for graphene formed on Ni(111). Here, however, the theoretical estimates of $|\delta_{LO}(\Gamma)|$ are underestimated.

Keywords: direct and indirect exchange, longitude optical frequency, SiC and d-metal substrates.

1. Introduction

There are three main channels for interaction of atoms adsorbed on metal and semiconductor substrates [1,2]: (*a*) dipole-dipole interaction and (*b*) direct and (*c*) indirect electron exchange. The dipole-dipole interaction is observed if charge transfer proceeds between adatoms and a substrate. The direct electron exchange arises at high concentrations of adatoms when the electron shells of nearest neighbors start to overlap. The indirect exchange is supported by virtual transitions of electrons between adatoms via the substrate states, which makes it similar to the RKKY (Ruderman−Kittel−Kasuya−Yosida) interaction. Interactions (*a*) and (*c*) are long-range ones, while interaction (*b*) is short-range. In the present paper, we examine how the characteristic frequencies of epitaxial graphene (epigraphene, or EPG) change relative to the frequencies of free-standing graphene (FSG) after the introduction of indirect interaction of carbon atoms in EPG. Note that the number of studies on the influence of a substrate on the phonon spectrum of epitaxial nanolayers is an order of magnitude lower than the number of similar studies on the electron spectrum [3].

The majority of experiments with EPG on semiconductors involve Raman spectroscopy [4–9]. At present, the experimenters believe that the red shift of the Raman G-peak[1] of EPG on semiconductors relative to the FSG G-peak is caused by elastic strain at the interface or the mismatch of coefficients of thermal expansion of the

epitaxial layer and the substrate (see [10] for a brief history of this interpretation and a critical review of it). However, we believe that the red shift of the G-peak of EPG is caused by the very interaction of the epilayer with the substrate and emerges regardless of the presence of mechanical stress at the interface. The validity of this statement was demonstrated in [10] within a model of two coupled oscillators. The authors of [11] examined the problem of G-peak shift within a more complex model of an epitaxial monolayer and a substrate crystallographically identical to it, which excludes the possibility of strain at the interface.

HREELS (high-resolution electron energy loss spectroscopy) and IHAS (inelastic helium atom scattering) methods were used to study the phonon spectrum of EPG formed on a metal substrate [12]. Unlike a graphene−semiconductor structure, graphene on a metal may exhibit softening of phonon modes.

The goal of the present study is to demonstrate that it is the indirect interaction that specifies both the sign and the magnitude of shift of phonon frequencies of EPG.

2. Problem of an adsorbed dimer

Let us start with discussing an auxiliary problem of two identical interacting atoms adsorbed on a semiconductor substrate. In the spinless approximation, the Hamiltonian

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[1] The FSG G-peak frequency corresponds to long-wave optical mode $\omega_{LO}(\Gamma)$ wherein graphene sublattices shift relative to each other.

of such a dimer is

$$H_{\text{dim}} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^{+} c_{\mathbf{k}} + \sum_{i=1}^{2} \varepsilon_i a_i^{+} a_i - t(a_1^{+} a_2 + a_2^{+} a_1)$$
$$+ \sum_{\mathbf{k},i} V_{\mathbf{k},i} (a_i^{+} c_{\mathbf{k}} + c_{\mathbf{k}}^{+} a_i). \qquad (1)$$

Here, $\varepsilon_{\mathbf{k},\nu}$ is the law of electron dispersion in the substrate, $\mathbf{k}$ is the wave vector comprising the band index, $c_{\mathbf{k}}^{+} (c_{\mathbf{k}})$ is the operator of electron creation (annihilation) in state $|\mathbf{k}\rangle$, $\varepsilon_{1(2)}$ is the energy of the $|p\rangle$-state of carbon atom 1 (2), $\varepsilon_1 = \varepsilon_2 = \varepsilon_p$, $a_{1(2)}^{+} (a_{1(2)})$ is the operator of electron creation (annihilation) in state $|p\rangle$ at atom 1 (2), t is the energy of electron transition between the $|p\rangle$-states of atoms 1 and 2 (direct kinetic exchange), and $V_{\mathbf{k},i}$ is the matrix element of electron transition between the $|p\rangle$-state of atom i and state $|\mathbf{k}\rangle$ of the substrate; $V_{\mathbf{k},1} = \exp(i\mathbf{k}r_{12})V_{\mathbf{k},2}$ for atoms at distance r_{12}. Using the approach and results of [13,14], we obtain the following Green's function:

$$G_{\text{dim}}(\varepsilon) = \left(\varepsilon - E(\varepsilon) + i\Gamma(\varepsilon) - \frac{(t - t_{\text{ind}}(\varepsilon))(t - t_{\text{ind}}^{*}(\varepsilon))}{\varepsilon - E(\varepsilon) + i\Gamma(\varepsilon)} \right)^{-1}. \qquad (2)$$

Here, ω is the energy variable; $\Gamma(\varepsilon) = \pi|V_{\mathbf{k},i}|^2 \rho_{\text{sub}}(\varepsilon)$ is the broadening function of state $|p\rangle$ of an adatom due to its interaction with a substrate with density of states $\rho_{\text{sub}}(\varepsilon)$; $E(\varepsilon) = \varepsilon_p + \Lambda(\varepsilon)$ is the adatom state energy; $\Lambda(\varepsilon)$ is the function of shift of state $|p\rangle$ with energy ε_p, which is a Hilbert transform of function $\Gamma(\varepsilon)$ [1,13–15], due to the interaction with the substrate; and the function of indirect interaction is

$$t_{\text{ind}}(\varepsilon) = V^2 \operatorname{Re} \sum_{\mathbf{k}} \frac{\exp(i\mathbf{k}r_{12})}{\varepsilon - \varepsilon_{\mathbf{k}} + i0^{+}}, \qquad (3)$$

where $V^2 = \langle |V_{\mathbf{k}i}|^2 \rangle_{\text{BZ}}$ and $\langle \ldots \rangle_{\text{BZ}}$ denotes averaging over the Brillouin zone of the substrate [1,13].

3. Graphene on a semiconductor

Since a metal substrate has already been analyzed in [13], let us examine a semiconductor substrate with the use of a simple model representing its conduction band C (valence band V) $\varepsilon_{\mathbf{k}}^{\text{C,V}}$ in the following way:

$$\varepsilon_{\mathbf{k}}^{\text{C,V}} = \pm \left(\frac{E_g}{2} + \frac{\hbar^2 k^2}{2m_{\text{C,V}}} \right), \qquad (4)$$

where E_g is the bandgap (the energy is measured from its center) and $m_{\text{C,V}}$ is the effective mass of an electron in the conduction band (valence band). Capitalizing on the results reported in [16] (see Appendix II), we obtain the following

for the substrate bandgap region $|\varepsilon| \leq E_g/2$:

$$t_{\text{ind}}^{\text{C,V}}(\mu) \approx -\frac{V^2 a^2 m_{\text{C,V}}}{\pi\hbar^2} \exp(-\kappa_{\text{C,V}} a),$$
$$\kappa_{\text{C(V)}} = \sqrt{2m_{\text{C,V}}|\Omega_{\text{C,V}}|}/\hbar, \qquad (5)$$

where $a = |\mathbf{r}_{12}| = 1.42\,\text{Å}$ is the distance between nearest neighbors in graphene, μ is the chemical potential set by the substrate, $\Omega_{\text{C}} = \mu - E_g/2 > 0$, $\Omega_{\text{V}} = \mu + E_g/2 < 0$, and $\hbar$ is the reduced Planck constant. To obtain order-of-magnitude estimates, we set $m_{\text{C}} = m_{\text{V}} = m^{*}$. Renormalized exchange interaction $\tilde{t}(\mu) = t - t_{\text{ind}}(\mu)$ may be rewritten as $\tilde{t}(\mu) = t(1 + \delta(\mu))$, $\delta(\mu) = -t_{\text{ind}}(\mu)/t > 0$. Introducing parameter $\kappa = \sqrt{2m^{*}|\Omega|}/\hbar$, where $\Omega = \mu + E_g/2$ and $|\mu| \leq E_g/2$, we find

$$t_{\text{ind}} \approx -(V^2 m^{*}/\pi\hbar^2) \exp(-\kappa a). \qquad (6)$$

At $\mu = 0$, we obtain maximum value $\kappa_{\text{max}} = \sqrt{m^{*} E_g}/\hbar \approx 0.63\,\text{Å}^{-1}$ (the use of (5) here is an extrapolation, since formula (5) was derived from (3) by the saddle-point method (see [16]) under the assumption that $a \gg 1$). At $m^{*} = m_0$ (m_0 is the mass of a free electron) and $E_g = 3\,\text{eV}$ (polytype 6*H*-SiC), we find $\kappa_{\text{max}} a \approx 0.89$. Note that the E_g values increase from 2.4 to 3.23 eV [17] in transition from cubic polytype 3*C*-SiC to hexagonal polytype 4*H*-SiC. Multiplier $\exp(\kappa_{\text{max}})$ decreases slightly (from 0.45 to 0.40) in this case. Using the Harrison bonding orbitals model (simplified method of linear combinations of atomic orbitals with a simple scheme of matrix elements calculation) [18,19], the authors of [20] obtained $t \approx 12\,\text{eV}$, where $t = V_{(\text{sp}^3/\text{sp}^3)\sigma}$ is the matrix element of σ-bonding of $|\text{sp}^3\rangle$-orbitals of neighboring graphene atoms, which is equal to 2 eV at an adsorption bond length of 3 Å [21] (here and elsewhere, all matrix elements of bonds are assumed to be positive). Then, $t_{\text{ind}} \approx 0.1-0.3\,\text{eV}$, and $\delta(0) \approx 0.1-0.3$ is obtained at $\mu \approx 0$.

Let us now turn to evaluating the effect of indirect exchange on the force constants and frequencies of epigraphene. The formulae for force constants of central α and non-central β interaction of nearest neighbors in graphene were obtained in [21]. In the context of the considered problem, they may be re-written as $\tilde{\alpha} = 4\tilde{t}/a^2$ and $\tilde{\beta} = (\tilde{\lambda}/3)\tilde{\alpha}$, where the metallicity effects were omitted for simplicity and $\tilde{\alpha}$ is a coefficient emerging due to the introduction of disorientation (reduction of overlapping) of $|\text{sp}^3\rangle$-orbitals of neighboring atoms involved in σ-bonding. This coefficient is 0.66 for graphene (and 0.85 for diamond [19]). Thus, we obtain

$$\tilde{\alpha} = \alpha(1 + \Delta\alpha/\alpha), \quad \tilde{\beta} = \beta(1 + \Delta\beta/\beta), \qquad (7)$$

where

$$\Delta\alpha = \frac{4\Delta t}{a^2} \quad \text{and} \quad \Delta\beta = (\tilde{\lambda}/3)\Delta\alpha.$$

It is evident that $\Delta\alpha/\alpha = \Delta\beta/\beta = -\delta$. According to [19], $\alpha \approx 22\,\text{eV/Å}^2$ and $\beta \approx 5\,\text{eV/Å}^2$. The values of

$\alpha \approx 17.6\,\text{eV/Å}^2$ and $\beta \approx 5\,\text{eV/Å}^2$ were obtained in [22] for the same force constants by fitting to experimental frequencies at points Γ and K of the Brillouin zone of graphene. (Strictly speaking, this comparison of non-central interaction constants is not quite correct, since constant β is associated with the disorientation of sp^2-orbitals of neighboring atoms forming a σ-bond (model of a rigid hexagon) in [21] and with a change in angle between sp^2-orbitals centered at one atom (model of angular stiffnesses) in [22].)

At $\alpha \approx 22\,\text{eV/Å}^2$, we obtain $\omega_{\text{LO}}(\Gamma) \approx 1700\,\text{cm}^{-1}$, which exceeds significantly the experimental values of G-peak frequencies $1565-1590\,\text{cm}^{-1}$ (see the references in [22]). However, it should be stressed that we did not perform fitting. In the case of FSG, we find 1380 and $1060\,\text{cm}^{-1}$ for optical phonons at point K (the values of 1195 and $1047\,\text{cm}^{-1}$ were given in [22]).

Let us introduce relative G-peak shift

$$\delta_{\text{G-peak}} = \Delta_{\text{G-peak}}/[\omega_{\text{LO}}(\Gamma)]_{\text{FSG}}, \qquad (8)$$

where

$$\Delta_{\text{G-peak}} = [\omega_{\text{LO}}(\Gamma)]_{\text{EPG}} - [\omega_{\text{LO}}(\Gamma)]_{\text{FSG}} > 0.$$

(Since $\Delta_{\text{G-peak}} > 0$, the G-peak is redshifted). According to [23], the following is true for graphene on a Si face of n-type polytype $6H$-SiC:

$$[\omega_{\text{LO}}(\Gamma)]_{\text{FSG}} = 1580\,\text{cm}^{-1}, \quad [\omega_{\text{LO}}(\Gamma)]_{\text{EPG}} = 1597\,\text{cm}^{-1},$$

which gives $\delta_{\text{G-peak}} \approx 0.01$. Since $[\omega_{\text{LO}}(\Gamma)]_{\text{EPG}} \propto \sqrt{\alpha}$, we obtain $\delta_{\text{G-peak}} = -\delta(0)/2 \sim 0.01$. However, this match between the obtained theoretical estimate and experimental data should not be overemphasized. The thing is that the value of parameter $V = \langle|V_{\mathbf{k}i}|^2\rangle_{\text{BZ}}^{1/2}$ is fairly hard to determine (see, for example, [24,25]), and V is often treated as a fitting parameter.

The results reported in [26], where an analytical expression for density of phonon states $\rho_{\text{ph}}(\omega)$ of graphene (see also formula (14) and Fig. 5 in [27]) was obtained, make it easy to demonstrate that $\rho_{\text{ph}}(\omega)$ changes by $\delta(0) \sim 0.01-0.03$ after the introduction of indirect interaction. This has virtually no effect on the thermal characteristics of graphene.

Let us consider certain anharmonic characteristics of the relative G-peak shift. It was demonstrated in [11] that the dependences of central interaction constant α on hydrostatic pressure P applied to graphene (i.e., on omnidirectional tension or compression) and temperature T may be presented in the following way:

$$\alpha(P) = \alpha(0) + \lambda_P P \text{ and } \alpha(T) = \alpha(0) - \lambda_T T,$$

where coefficients λ_P and λ_T are positive. The G-peak frequency shift is then

$$\Delta_{\text{LO}}(P) = c_1 + c_2 P, \quad \Delta_{\text{LO}}(T) = c_3 - c_4 T,$$

where all c_i are positive (see references to the corresponding experimental data in [11]). Since distance a between

nearest neighbors in graphene decreases with increasing P, the contribution of indirect exchange $|t_{\text{ind}}| \propto \exp(-\kappa a)$ increases (see (6)). It follows that the introduction of indirect interaction leads to an increase in coefficient λ_P and constant c_2. The value of a increases with increasing T, thus reducing coefficient λ_T and constant c_4. However, it should be noted that $(\partial E_g)/\partial T < 0$ [28] for the vast majority of semiconductors (SiC polytypes included [29]), and this compensates for the λ_T and c_4 reduction to a certain extent. Expressions for the force constants with anharmonicity were obtained within the Harrison bonding orbitals model in [30].

4. Graphene on a d-metal

Let us now consider graphene formed on metal substrates, which has enjoyed increased interest in recent years [12,31]. It turned out that, among other things, even a slight variation of binding between a metal and graphene leads to a significant alteration of the phonon spectrum of the latter; therefore, one may probe the metal−graphene bond by measuring the corresponding phonon shifts, which is of interest for flexible electronics and plasmonics [12].

In the case of EPG on a metal, we obtain the following expression instead of (6):

$$t_{\text{ind}}^{\text{met}}(\mu) \approx -\frac{V^2 a^2 m^*}{\pi\hbar^2}\cos(ak_{\text{met}}^*), \quad k_{\text{met}}^* = \sqrt{2m^*\mu}/\hbar, \quad (9)$$

where energy μ is measured from the bottom of the conduction band of this metal with dispersion law $\varepsilon_{\mathbf{k}}^{\text{met}} = \hbar^2 k^2/2m^*$. If $\mu < \bar{\mu} = 1/(8m^*)\pi^2\hbar^2/a^2$, we have $\cos(ak_{\text{met}}) > 0$ and $\delta(\mu) > 0$; if $\mu > \bar{\mu}$, $\delta(\mu) < 0$. At $m^* = m_0$, we obtain $\bar{\mu} \approx 4.7\,\text{eV}$, which exceeds width W_d of d-bands for Co, Ni, Cu, and Ag [18]. Therefore, $\cos(ak_{\text{met}}) < 0$ for graphene formed on these metals. It follows that $\delta(\mu) = -t_{\text{ind}}/t < 0$; i.e., the interatomic binding in graphene gets weaker, and mode $\omega_{\text{LO}}(\Gamma)$ of epigraphene softens accordingly. It is assumed that $V = V_{\text{pd}\sigma}$, where

$$V_{\text{pd}\sigma} = \frac{3\sqrt{15}}{2\pi}[(\hbar^2/m_0)(r_p r_d^3)^{1/2}]/d^4, \qquad (10)$$

r_d and r_p are the radii of $|d\rangle$- and $|p\rangle$-states ($r_p = 6.59\,\text{Å}$ for a carbon atom) and d is the length of the bond between a graphene atom and a d-metal atom [32]. The input parameters and the results of calculation for cobalt, nickel (strong bond with graphene), and copper (weak bond with graphene) substrates are presented in the table [12].

Let us determine the values of multipliers $\cos(ak_{\text{met}}^0)$, where $k_{\text{met}}^0 = \sqrt{2m_0\mu}/\hbar$, and $\cos(ak_{\text{met}}^*)$. Relying on the Friedel model of the density of states of the d-band with $\rho_d(\varepsilon) = 10/W_d$ at $-W_d/2 \le \varepsilon \le W_d/2$ and $\rho_d(\varepsilon) = 0$ at $|\varepsilon| > W_d/2$ [18,34], we obtain $\mu = N_d W_d/10$, where number N_d of electrons in a metal is set to 8, 9, and 10 for Co, Ni, and Cu, respectively (more accurate values of N_d were given in [35]). Introducing ratio $\nu = m^*/m_0$, where m^* is the effective mass of d-electrons, we obtain the

Values of metal−graphene distance d, radius r_d of the d-state, ratio $v = m^*/m_0$, and the cosine in expression (9)

Parameters		Metal		
		Co	Ni	Cu
d, Å[12]		2.1	20.1	3.3
r_d, Å[18]		0.76	0.71	0.67
V, eV		2.77	2.77	0.65
$\cos(ak^0_{\text{met}})$ $(v = 1)$		0.57	0.58	0.65
[33]	v	2.07	1.82	1
	$\cos(ak^*_{\text{met}})$	0.06	0.28	0.65
Calculation	v	3.51	3.36	3.27
	$\cos(ak^*_{\text{met}})$	−0.23	−0.17	0.02

results presented in the table. It follows from the table that $t^{\text{met}}_{\text{ind}}(\mu) < 0$ at $v = 1$, which implies an increase in frequency $\omega_{\text{LO}}(\Gamma)$ in EPG relative to FSG. In the case of cobalt and nickel substrates, we find $t^{\text{met}}_{\text{ind}}(\mu) > 0$ at large values of m^*. It follows that the indirect interaction of graphene atoms in EPG leads to softening of frequencies $\omega_{\text{LO}}(\Gamma)$.

Let us turn to the experimental data for the most thoroughly studied structure: graphene on Ni(111) [12,35–37] (this is the nickel face on which quasi-free graphene has been grown for the first time). Note also that the mismatch of lattices in this structure is below 2% (the same is true for Co(0001)). As was demonstrated in [37], shift $\Delta\omega_{\text{LO}}(\Gamma) \approx -(70-100)\,\text{cm}^{-1}$; thus, the relative softening of mode $\omega_{\text{LO}}(\Gamma)$ is $\delta\omega_{\text{LO}}(\Gamma) \approx -(0.04-0.06)$. Introducing $\delta_{\text{met}} = t^{\text{met}}_{\text{ind}}/t$, we obtain -0.03 at $v = 3.36$. Thus, the obtained estimate $\delta\omega_{\text{LO}}(\Gamma) = \delta_{\text{met}}/2$ is several times lower in magnitude than the experimental value.

5. Conclusion

It was demonstrated that the direction and magnitude $\Delta_{\text{G-peak}}$ of red shift of the G-peakt of epitaxial graphene is related to the enhancement of interaction of neighboring graphene atoms due to indirect virtual electron exchange via the substrate. Thus, the measurement of $\Delta_{\text{G-peak}}$ provides data on the magnitude of indirect exchange relative to the direct one $(|t_{\text{ind}}|/t)$ rather than on the stress induced in graphene as a result of contact with a substrate (see references to such studies in [11]). In the present study, we limited ourselves to rather crude band models and extrapolations (6) and (9), since the goal was to obtain qualitative results (specifically, identify the factor that governs the sign and magnitude of $\Delta_{\text{G-peak}}$). The key finding is that the indirect exchange of graphene adatoms is the factor inducing shift $\Delta\omega_{\text{LO}}(\Gamma)$ of frequency $\omega_{\text{LO}}(\Gamma)$. Theory provides a fairly adequate description of both the direction and the magnitude of $\Delta\omega_{\text{LO}}(\Gamma)$ (red shift of the G-peak) for

graphene on a silicon carbide polytype. As for graphene on d-metals, we are able to demonstrate that $\Delta\omega_{\text{LO}}(\Gamma) < 0$ (blue shift) is feasible only for metals with narrow d-bands or large effective masses (i.e., metals at the end of the $3d$-series). However, the $|\Delta\omega_{\text{LO}}(\Gamma)|$ magnitude is several times lower than the one observed in experiments. This is hardly surprising, since the Harrison bonding orbitals model was originally developed specifically for semiconductors. In summary, it can be said that we managed to demonstrate in a fairly convincing manner that the indirect exchange is the factor responsible for key differences between the phonon spectra of FSG and EPG.

Conflict of interest

The author declares that he has no conflict of interest.

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