Publ. Astron. Obs. Belgrade No. 102 (2022), 117 - 120 *Contributed Paper*

ANALYTICAL EXPRESSION FOR STOPPING FORCE ACTING ON A SLOW CHARGED PARTICLE MOVING PARALLEL TO A THICK GRAPHENE-SAPPHIRE-GRAPHENE STRUCTURE

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Abstract. We derive an analytical expression for the stopping force acting on an external charged particle moving parallel to a sandwich-like structure consisting of two undoped graphene sheets separated by a layer of Al_2O_3 (sapphire).

1. INTRODUCTION

Experimental designs of nanoscale devices involving graphene require stacking of graphene layers with insulating spacer layers (Yan et al. 2012), which usually support strong Fuchs-Kliewer (FK) or optical surface phonon modes (Fischetti et al. 2001). In our previous publication (Despoja et al. 2017), as a prototype of layered heterostructures involving graphene sheets, we have studied a graphene-Al_2O_3-graphene (for short, denoted by gr-Al_2O_3-gr) composite system and derived an expression for its effective dielectric function. In the following papers (Despoja et al. 2019 and Kalinić et al. 2021), the wake potential produced by an external charged particle that moves parallel to a sandwich-like gr-Al_2O_3-gr structure was investigated. We have found that in a low-velocity regime (below the threshold for excitations of the Dirac plasmon in graphene, given by its Fermi velocity v_F) only the transverse optical (TO) phonons in the Al_2O_3 layer contribute to the wake potential in the plane of the graphene layer closest to the incident particle. Finally, in our recent publication (Kalinić et al. 2020) we have derived general expressions for the stopping and image forces acting on the external charged particle moving parallel to the gr-Al_2O_3-gr composite. In this work, in order to provide an analytical estimate of the peak in the stopping force in the range of speeds below v_F, we analytically evaluate the stopping force on the external charged particle moving parallel to two undoped graphene layers with Al_2O_3 in between. Note that we use Gaussian electrostatic units, set $\hbar = 1$, and denote the charge of a proton by $e > 0$.

2. BASIC THEORY

We use a Cartesian coordinate system with coordinates $\{\vec{R}, z\}$, where $\vec{R} = \{x, y\}$ is a two-dimensional (2D) position vector in the xy-plane and z is the distance from it. Two graphene sheets are placed in the planes $z = \pm a/2$, with the space between them being a layer of Al_2O_3 (sapphire) of thickness a. Assuming that the layered structure is translationally invariant in the xy directions, we perform a 2D spatial ($\vec{R} \rightarrow \vec{q}$) and a temporal ($t \rightarrow \omega$) Fourier transform of all relevant quantities. The sapphire layer is approximated by a homogeneous dielectric slab described by local dielectric function $\varepsilon_s(\omega)$, whereas bottom and top graphene sheets are described by the 2D response functions $\chi_1(q, \omega)$ and $\chi_2(q, \omega)$, respectively. The entire system is assumed to be in vacuum or air.

The stopping force acting on the external point charge Ze moving parallel to a gr-Al_2O_3-gr composite at a fixed distance b above the top graphene layer with a constant velocity v may be expressed as (Preciado Rivas et al. 2021)

$$\mathrm{F}_s = -\frac{2(Ze)^2}{\pi v} \int_0^\infty e^{-2qb} dq \int_0^{qv} \frac{\omega}{\sqrt{(qv)^2 - \omega^2}} Im\left[-\frac{1}{\varepsilon(q,\omega)}\right] d\omega \tag{1}$$

where the effective 2D dielectric function $\varepsilon(q, \omega)$ is given by (Despoja et al. 2017)

$$\varepsilon(q,\omega) = \frac{1}{2}\left[1 + \varepsilon_s(\omega)\coth(qa) + \frac{4\pi e^2}{q}\chi_2\right] - \frac{1}{2}\frac{\varepsilon_s^2(\omega) cosech^2(qa)}{1 + \varepsilon_s(\omega)\coth(qa) + \frac{4\pi e^2}{q}\chi_1} \tag{2}$$

It is shown (Kalinić et al. 2022) that, for the choice of the parameters $a \gg b$, the two surfaces of our sandwich-like structure are electrostatically decoupled. Mathematically, this occurs when $qa \gg 1$. Then, setting $\coth(qa) \approx 1$ and $cosech(qa) \approx 0$ in Eq. (2) one obtains an effective dielectric function for a singlelayer graphene with polarization χ_2 deposited on a semi-infinite substrate with the dielectric permittivity ε_s

$$\varepsilon(q,\omega) = \frac{1}{2}\left[1 + \varepsilon_s(\omega) + \frac{4\pi e^2}{q}\chi_2\right] \tag{3}$$

Since we are interested in low speeds, we may approximate the response function of the top graphene layer by its static limit. For an undoped graphene, this gives $\chi_2 \approx q/(4v_F)$. In that case, Eq. (3) may be approximated as

$$\varepsilon(\omega) \approx \frac{1}{2}\left[1 + \varepsilon_s(\omega) + \frac{\pi e^2}{v_F}\right] \tag{4}$$

As a result, the energy loss function (ELF) in Eq. (1), $Im[-1/\varepsilon(q,\omega)]$, becomes independent of q and it features sharp peaks at frequencies corresponding to the FK phonons in the Al_2O_3 substrate, modified by the static screening by graphene. By solving the equation $\varepsilon(\omega) = 0$, and taking the expression for $\varepsilon_s(\omega)$ (Fischetti et al. 2001) which includes two TO phonon modes at 48 meV and 71 meV with zero damping, one obtains the screened FK phonon frequencies in the Al_2O_3 substrate as $\omega_{FK1} \approx 54$ meV and $\omega_{FK2} \approx 86$ meV. Thus, we may approximate the ELF in Eq. (1) by (Preciado Rivas et al. 2021)

$$Im\left[-\frac{1}{\varepsilon(\omega)}\right] \approx \sum_{i=1}^{2} A_i \delta(\omega - \omega_{FKi}) \tag{5}$$

with the weight constants $A_i = \pi/|\varepsilon'(\omega_{FKi})|$, which take values $A_1 \approx 1.5$ meV and $A_2 \approx 8.8$ meV.

Substituting Eq. (5) into Eq. (1) one obtains an analytical approximation as

$$\mathrm{F}_s \approx -\frac{2(Ze)^2}{\pi v^2}\sum_{i=1}^{2} A_i \omega_{FKi} K_0\left(2\frac{b}{v}\omega_{FKi}\right) \tag{6}$$

where K_0 is a Bessel function.

3. RESULTS AND DISCUSSION

In Fig. 1 we show the four stopping forces in the range of speeds from 0 to $0.9v_F$ for two undoped graphene sheets [Fermi energy is $E_F = 0$, marked as gr(0)] a distance $a = 5$ nm apart with the Al_2O_3 layer in between, using the particle distance $b = 0.5$ nm: F_s is evaluated from Eq. (1) using Eq. (2) and the dynamic polarization function of graphene within the random phase approximation for its π bands; $F_s^{(1+2)}$, $F_s^{(1)}$, and $F_s^{(2)}$ are evaluated from Eq. (6) for both FK phonons, only for ω_{FK1}, and only for ω_{FK2}, respectively. It is evident that analytical expression for the stopping force well reproduces the peak at $v \approx 0.08v_F$, showing that its origin is dominantly in the phonon mode in the Al_2O_3 surface with ω_{FK2}.

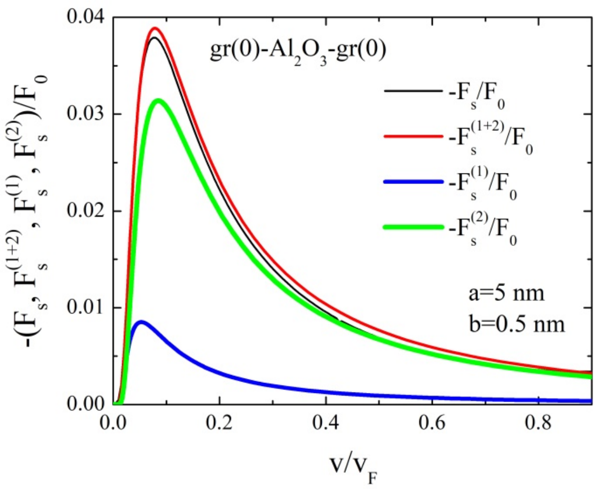

Figure 1: The stopping forces: F_s (thin black line), $F_s^{(1+2)}$ (medium red line), $F_s^{(1)}$ (thick blue line), and $F_s^{(2)}$ (extra thick green line), normalized by $F_0 = [Ze/(2b)]^2$, as functions of the speed v (normalized by v_F) of a proton ($Z = 1$) moving at a distance $b = 0.5$ nm above two undoped graphene sheets with Al_2O_3 in between. The separation between graphene layers (or the Al_2O_3 slab thickness) is $a = 5$ nm.

Acknowledgments

This research is funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia, the Croatian Science Foundation (Grant No. IP-2020-02-5556), the European Regional Development Fund for the 'QuantiXLie Centre of Excellence' (Grant No. KK.01.1.1.01.0004), and the Natural Sciences and Engineering Research Council of Canada (Grant No. 2016-03689).

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