Theoretical investigation of the interaction of charged particle beams with carbon nanostructures

I. Radović*, T. Djordjević, D. Borka
Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

L. Karbunar
School of Electrical Engineering, University of Belgrade, Bulevar Kralja Aleksandra 73, 11120 Belgrade, Serbia

Z.L. Mišković
Department of Applied Mathematics, and Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

Firstly, we use the dielectric-response formalism for graphene’s π-electron bands in the random phase approximation (RPA) [1] to show how an incident charged particle may be used to probe the hybridization taking place between the Dirac plasmon in graphene and the surface optical phonon modes in a SiO₂ substrate. A low-frequency collective mode resulting from this hybridization may be excited by matching its phase velocity with the ion speed lower than the graphene Fermi speed [2]. Strong effects of this hybridization are found in the wake pattern in the induced potential, as well as in the stopping and image forces that act on the incident charge in a broad range of its velocities, in a manner that may be controlled by changing the doping density of graphene [3].

Secondly, we present a theoretical modeling of the experimental electron energy loss spectra of freestanding films consisting of N graphene layers in a scanning transmission electron microscope [4]. Using a two-dimensional (2D), two-fluid hydrodynamic (2FHD) model for the single-layer polarizability, we find good agreement (as shown in Fig. 1) with the experimental data [5].

Finally, we present a theoretical modeling of the energy-loss spectroscopy data for monolayer graphene supported by Pt(111), Ru(0001) and Ni(111) substrates [6]. To reproduce the experimental loss function, we use a 2D, 2FHD model for interband transitions of graphene’s π and σ electrons and an empirical Drude-Lorentz model in the local approximation for metal substrates.

![Figure 1: Probability density P(ω) (in 1/eV) versus energy loss ω (in eV), evaluated for N=1, 2, 5, and 13 graphene layers [4] [smooth solid (yellow, green, blue, and pink) curves], along with the corresponding experimental EEL spectra [5] [noisy (gray) curves].](image)

References


*iradovic@vin.bg.ac.rs