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Image potential and stopping force in the interaction of fast ions with carbon nanotubes: The extended two-fluid hydrodynamic model

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ABSTRACT

We study the interaction of charged particles with a (6, 4) single-walled carbon nanotube (SWNT) under channeling conditions by means of the linearized, two dimensional (2D), two-fluid extended hydrodynamic model. We use the model to calculate analytically and numerically the image potential and the stopping force for a proton moving parallel to the axis of the SWNT, both inside and outside the nanotube at the speeds from 0.5 a.u. to 15 a.u. The effects of different angular modes on the velocity dependence of the image potential are compared for a proton moving in different types of SWNTs. We also compute the spatial and angular distributions of protons in the 2D two-fluid extended hydrodynamic model and compare them with the 2D two-fluid hydrodynamic model with zero damping.

1. Introduction

Carbon nanotubes were discovered in the beginning of 1990s [1]. They can be described as sheets of carbon atoms at the (two-dimensional) hexagonal lattice sites rolled up into cylinders [2]. Soon after the discovery of carbon nanotubes, Klimov and Letokhov [3] realized that the effect of channeling of positively charged particles in nanotubes might occur. After that, a number of theoretical groups have studied ion channeling in nanotubes [4–12], with the main objective to explore the possibility of guiding charged-particle beams with nanotubes. Because of technical problems that involve ordering, straightening and holding nanotubes, the experimental study of ion channeling through carbon nanotubes is still in the initial phase [13,14].

For ion channeling in carbon nanotubes at the low (<100 keV) and high (>10 MeV) ends of the energy range, the dynamic polarization effect of valence electrons in the nanotubes can be omitted. However, ions moving with the energies (100 keV–10 MeV) will induce strong dynamic polarization of valence electrons in the nanotubes which in turn will give rise to a sizeable image force on the ions, as well as a considerable energy loss due to the collective, or plasma, electron excitations [15–17]. The dynamic image force obtained from a one-fluid hydrodynamic model was shown to have big influence in the angular distributions of protons channeled through short (11, 9) single-wall carbon nanotubes [18] in vacuum. However, in Ref. [19] we treated the σ and π electron orbitals in carbon nanostructures as separate but superimposed fluids with zero restoring frequencies and zero damping and calculated the image force and stopping force based on a 2D two-fluid hydrodynamic model. We found that those forces are affected, both at the low and high proton speeds, by a splitting of the collective electron excitation modes occurring due to different acoustic speeds in the σ and π electron fluids that may be related to the so-called high-energy $\sigma+\pi$ plasmons and the low-energy π plasmons [17,19]. In this work, we use a more realistic approach for calculations of the image potential and stopping force based on a 2D two-fluid hydrodynamic model, which includes finite restoring frequencies and finite damping of the σ and π electron that are determined from the EELS measurements [20]. Hence, we designate such version of the two-fluid hydrodynamic model as *extended* in contrast to the previously used two-fluid hydrodynamic model, which will be understood as having zero restoring frequencies and zero damping of the collective modes [19].

This paper is a continuation of the investigations in our previous paper [19] where we studied the image potential in the interaction of fast ions with carbon nanotubes and made comparisons between the one-fluid and two-fluid hydrodynamic models. In this work we present the analytically and numerically calculated image potential and the stopping force in the case of a 2D two-fluid extended hydrodynamic model [20]. We suppose that protons move parallel to the axis of the SWNTs at the speeds from 0.5 a.u. to 15 a.u. We investigate the cases when the particle position

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is inside and also outside the nanotube. We analyze the effects of different values of the angular mode on the velocity dependence of the reduced image potential for a proton moving in the SWNT, and we compare those effects for different types of nanotubes (SWNT (6, 4), SWNT (8, 6), SWNT (11, 9) and SWNT (15, 10)). We also compute the spatial and angular distributions of channeled protons using the two-fluid extended and the two-fluid hydrodynamic models [19,21,22]. First, we outline the basic theory used in modeling the image potential and stopping force of carbon nanotubes. After that, we discuss the obtained results for the image potential and stopping force, as well as the Monte Carlo simulations of spatial and angular distributions. At the end of the paper, we give our concluding remarks. Atomic units are used throughout unless explicitly stated otherwise.

2. Basic theory

A SWNT is modeled as an infinitesimally thin cylindrical shell with the radius R and the length L. We assume that the valence electrons in the ground state may be considered as a free-electron gas distributed uniformly over a cylindrical surface, with the number density per unit area $n_0 = n_\sigma^0 + n_\pi^0 = 0.428$ where $n_\sigma^0 = 3n_0/4 = 0.321$ and $n_\pi^0 = n_0/4 = 0.107$ are the unperturbed number densities corresponding to three σ electrons and one π electron per carbon atom, respectively [17]. We use cylindrical coordinates $\vec{r} = (\rho, \varphi, z)$ and assume that a charged particle with the charge Q moves outside the SWNT, with its trajectory parallel to the nanotube axis z, at fixed distance $\rho_0 > R$, such that the particle's instantaneous position is given by $\vec{r}_0(t) = (\rho_0, \varphi_0, vt)$, where v is the particle's speed.

The Fourier–Bessel (FB) transform $A(\rho, m, k, \omega)$ of an arbitrary function $A(\rho, \varphi, z, t)$ may be defined (assuming $L \to \infty$) by [19]

$$A(\rho,\varphi,z,t) = \frac{1}{(2\pi)^3}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(\rho,m,k,\omega)e^{im\varphi+ikz-i\omega t}dkd\omega \tag{1}$$

Following Ref. [19], one can express the induced potential Φ_{ind} due to dynamic polarization of the electron fluids as

$$\Phi_{ind}(\rho,m,k,\omega) = -2\pi RQ g_{mk}(\rho,R)g_{mk}(R,\rho_0)\chi(m,k,\omega)\delta(\omega - kv) \tag{2}$$

where $g_{mk}(\rho,R) = 4\pi I_m(|k|R)K_m(|k|\rho)$ and $g_{mk}(R,\rho_0) = 4\pi I_m(|k|R)\times K_m(|k|\rho_0)$, while I_m and K_m are cylindrical Bessel functions of integer order m, and the density response function of a carbon nanotube is given by

$$\chi(m,k,\omega) = \frac{\chi_0(m,k,\omega)}{1 + 4\pi RI_m(|k|R)K_m(|k|R)\chi_0(m,k,\omega)} \tag{3}$$

where the two-fluid extended non-interacting response function is given by $\chi_0(m,k,\omega) = \chi_\sigma^0(m,k,\omega) + \chi_\pi^0(m,k,\omega)$ with [23]

$$\chi_i^0(m,k,\omega) = \frac{n_i^0\left(k^2 + \frac{m^2}{R^2}\right)}{s_i^2\left(k^2 + \frac{m^2}{R^2}\right) + \omega_{ir}^2 - \omega^2 - i\gamma_i\omega} \tag{4}$$

Note that s_i, ω_{ir} and γ_i are the acoustic speed of the density perturbations of valence electrons (which is given in Ref. [23] in the Thomas–Fermi–Dirac approximation for the 2D hydrodynamic model), restoring frequency and the damping rate in the ith fluid (where the index i takes values σ and π), respectively. As regards the adjustable parameters in Eq. (4), we use $\omega_{\sigma r} = 0.48$, $\omega_{\pi r} = 0.15$, $\gamma_\sigma = 0.1$ and $\gamma_\pi = 0.09$. Those parameters are used in our previous publications devoted to modeling of the experimental electron energy loss (EEL) spectra of single-layer (SL) and multilayer graphene in a transmission electron microscope [20], and the high-resolution reflection EEL spectra of a SL graphene supported by a metal substrate [24]. Note that the previously used two-fluid hydrodynamic model is obtained by simply setting $\omega_{\sigma r}$, $\omega_{\pi r}$, γ_σ and γ_π to zero [19].

By using Eqs. (1) and (2) one can obtain an expression for the induced potential as follows

$$\Phi_{ind}(\rho,\varphi,z,t) = -4RQ\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} e^{im\varphi+ik(z-vt)}K_m(|k|\rho)K_m(|k|\rho_0) \times I_m^2(|k|R)\chi(m,k,kv)dk \tag{5}$$

The image potential, or the self energy, U_{im}, for a point-charge ion Q on the trajectory $\vec{r}_0(t) = (\rho_0, \varphi_0, vt)$ is defined by

$$U_{im} = \frac{Q}{2}\Phi_{ind}(\rho,\varphi,z,t)\Big|_{\rho=\rho_0,\ \varphi=\varphi_0,\ z=vt} \tag{6}$$

Substituting Eq. (5) into Eq. (6) and setting $\varphi_0 = 0$, it is easy to obtain the following relation for the image potential

$$U_{im} = -4Q^2R\sum_{m=-\infty}^{\infty}\int_0^{\infty} I_m^2(kR)K_m^2(k\rho_0)\mathrm{Re}[\chi(m,k,kv)]dk \tag{7}$$

where we have used the symmetry properties of the real and imaginary parts of the density response function of a carbon nanotube from Eq. (3).

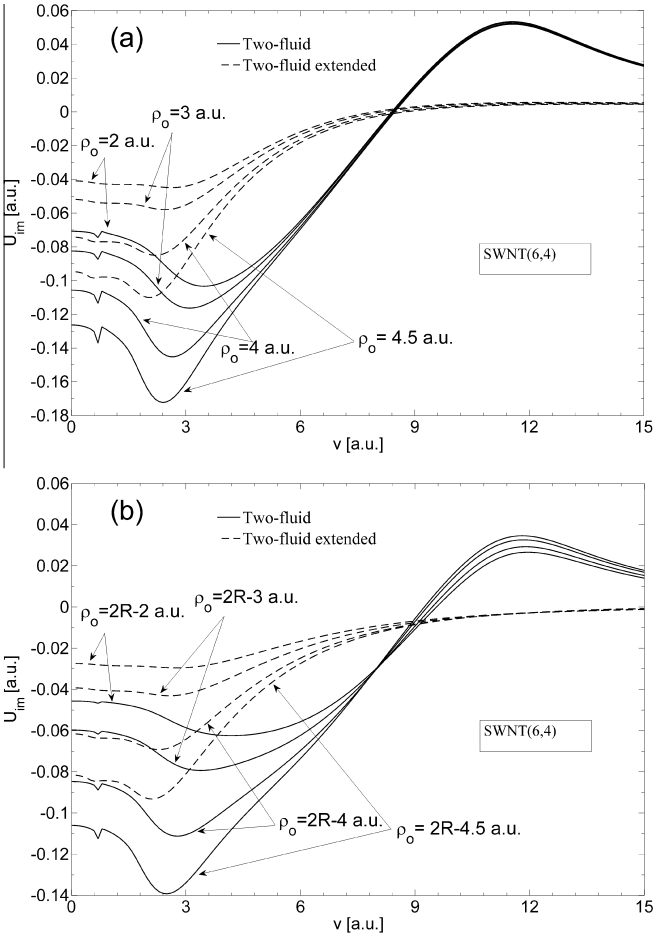

Fig. 1. Effects of the proton position ρ_0 on the velocity dependence of the image potential for a proton moving in the case of SWNT (6, 4) (a) inside and (b) outside the nanotube. The proton positions inside the nanotube are ρ_0 = 2, 3, 4 and 4.5 a.u., and outside the nanotube are ρ_0 = 2 R-2, 2 R-3, 2 R-4 and 2 R-4.5 a.u. Results are presented using two-fluid (solid curves) and two-fluid extended (dashed curves) hydrodynamic models. The nanotube radius of SWNT (6, 4) is R = 0.346 nm = 0.654 a.u.