Nuclear Instruments and Methods in Physics Research B 358 (2015) 82–87

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Image potential in the interaction of fast ions with carbon nanotubes: A comparison between the one- and two-fluid hydrodynamic models

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ARTICLE INFO

Article history:
Received 9 March 2015
Received in revised form 14 May 2015
Accepted 27 May 2015
Available online 10 June 2015

Keywords:
Nanotubes
Channeling
Dynamic polarization

ABSTRACT

We study the interaction of charged particles with four different types of single-walled carbon nanotubes (SWNTs) under channeling conditions by means of the linearized, two dimensional, one-fluid and two-fluid hydrodynamic models. The models are used to calculate the image potential for protons moving parallel to the axis of the SWNTs at the speeds up to 10 a.u. Numerical results are obtained to show the influence of the damping factor, the nanotube radius, and the particle position on the image potential inside the nanotube. We also compute the spatial and angular distributions of protons and compare them for the two models.

1. Introduction

After the discovery of carbon nanotubes, there has been a growing interest in investigation of interactions of charged particles with the nanotubes. It has been demonstrated that one of the possible applications may be to use carbon nanotubes to efficiently guide charged-particle beams [1–10] in the way very similar to crystal channeling. However, the experimental study of ion channeling through carbon nanotubes is still in the initial phase. The most challenging task is to solve the problems of ordering, straightening and holding nanotubes. The first experimental data on ion channeling through nanotubes were reported by Zhu et al. [11]. The first experiment with guiding of electrons by nanotubes was performed by Chai et al. [12].

An ion that moves with medium (MeV) energy will induce a strong dynamic polarization of valence electrons in the nanotubes which in turn will give rise to a sizeable image force on the ion, as well as a considerable energy loss due to the collective, or plasma, excitations of those electrons [13–15]. The dynamic image force was shown to exert large influence in the angular distributions of protons channeled through short single-walled (11, 9) carbon nanotubes (SWNTs) [16] placed in vacuum. Calculations of the image force in Ref. [16] were based on a two-dimensional (2D), one-fluid hydrodynamic model, which treats all four valence electrons in carbon atoms as a single charged fluid occupying the surface of a cylinder. However, treating the σ and π electron orbitals in carbon nanostructures as separate but superimposed 2D fluids with their own internal interactions due to the Thomas–Fermi pressure and the quantum correction to the electron kinetic energy gives rise to splitting of the collective electron excitation modes into the so-called high-energy $\sigma+\pi$ plasmons and the low-energy π plasmons [15]. As a consequence of this plasmon splitting, one finds that differences also arise in both the stopping power [15] and the image potential [17] when the two-fluid model is used instead of the one-fluid model. Those differences are yet to be tested in the spectra of medium-energy ions channeled through SWNTs.

Therefore, in this work we continue investigation from previous papers [14–16] and compare one- and two-fluid hydrodynamic models for the dielectric response of nanotube electrons. We present a detailed derivation of the image potential in the case of a two-fluid hydrodynamic model and compute, for the first time, both the angular and spatial distributions of channeled protons using that model. A comparison is made with the distributions obtained using the image potential from the one-fluid model for protons moving parallel to the axes of the (6, 4), (8, 6), (11, 9) and (15, 10) SWNTs at the speeds up to 10 a.u. After outlining the basic theory used in modeling the dynamic polarization effects of carbon nanotubes and in proton channeling, we discuss the results of our ion trajectory simulations of angular and spatial distributions and give our concluding remarks. Atomic units are used throughout unless explicitly stated otherwise.

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http://dx.doi.org/10.1016/j.nimb.2015.05.041
0168-583X/

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 $n_0 = n_\sigma^0 + n_\pi^0$ where $n_\sigma^0 = 0.321$ and $n_\pi^0 = 0.107$ are the unperturbed number densities corresponding to three σ electrons and one π electron per carbon atom, respectively [15]. We use cylindrical coordinates $\vec{r} = (\rho, \varphi, z)$ and assume that an external point charge Q moves within the nanotube, with its trajectory parallel to the nanotube axis z, 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. Let $n_i(\vec{r}_s, t)$ be the first-order perturbation of the electron number density (per unit area) and $\vec{u}_i(\vec{r}_s, t)$ be the tangential velocity field in the ith fluid, where the index i takes values σ and π, and $\vec{r}_s = (\varphi, z)$ is the coordinate of a point at the cylindrical surface of the nanotube. Based on the linearized, 2D, two-fluid hydrodynamic model [15,17,18], the electronic excitations on the cylindrical surface for each fluid may be described by the continuity equation:

$$\frac{\partial n_i(\varphi, z, t)}{\partial t} + n_i^0 \nabla_{||} \cdot \vec{u}_i(\varphi, z, t) = 0, \tag{1}$$

and the momentum-balance equation,

$$\frac{\partial \vec{u}_i(\varphi, z, t)}{\partial t} = \nabla_{||}\Phi(\rho, \varphi, z, t)|_{\rho=R} - \frac{\alpha_i}{n_i^0}\nabla_{||} n_i(\varphi, z, t) + \frac{\beta}{n_i^0}\nabla_{||}\left[\nabla_{||}^2 n_i(\varphi, z, t)\right] - \gamma_i \vec{u}_i(\varphi, z, t). \tag{2}$$

Note that, in Eqs. (1) and (2), $\nabla_{||} = (1/R)\vec{e}_\varphi(\partial/\partial\varphi) + \vec{e}_z(\partial/\partial z)$ differentiates only tangentially to the nanotube surface [14]. The first term on the right-hand side of Eq. (2) is the force on an electron due to the tangential component of the electric field, evaluated at the nanotube surface, where $\Phi = \Phi_{ext} + \Phi_{ind}$ is the total electrostatic potential, which consists of the potential Φ_{ext} from the external point charge Q and the induced potential Φ_{ind} due to dynamic polarization of the electron fluids. The second term is the force due to the internal interactions in the ith electron fluid, with $\alpha_i \equiv \pi n_i^0$ being the square of the speed of propagation of the density disturbances in a 2D Fermi electron gas. The third term with $\beta = 1/4$ comes from the quantum correction for the kinetic energy in this gas. The last term on the right-hand side of Eq. (2) represents the frictional force on an electron due to scattering on the positive-charge background, with γ_i being the friction coefficient. In our calculations we shall assume $\gamma_\sigma = \gamma_\pi = \gamma$ and adopt $\gamma = 0.001$ as a standard value in the case of negligible damping.

By eliminating the velocity fields $\vec{u}_i(\varphi, z, t)$, one obtains from Eqs. (1) and (2):

$$\left(\frac{\partial^2}{\partial t^2} + \gamma_i\frac{\partial}{\partial t} - \alpha_i\nabla_{||}^2 + \beta\nabla_{||}^4\right) n_i(\varphi, z, t) = -n_i^0\nabla_{||}^2\Phi(\rho, \varphi, z, t)|_{\rho=R}. \tag{3}$$

Assuming $L \to \infty$ we may define the Fourier–Bessel (FB) transform $A(\rho, m, k, \omega)$ of an arbitrary function $A(\rho, \varphi, z, t)$, by [19]:

$$A(\rho, \varphi, z, t) = \frac{1}{(2\pi)^3}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(\rho, m, k, \omega)e^{im\varphi + ikz - i\omega t}dkd\omega. \tag{4}$$

Taking the FB transform of Eq. (3), we obtain a relation between the perturbed electron number density and the local value of the total electrostatic potential at the nanotube surface $\rho = R$ in the form

$$n(m, k, \omega) = \chi_0(m, k, \omega)\Phi(\rho, m, k, \omega)|_{\rho=R}, \tag{5}$$

where $n(m, k, \omega) = n_\sigma(m, k, \omega) + n_\pi(m, k, \omega)$ and the two-fluid response function is given by $\chi_0(m, k, \omega) = \chi_\sigma^0(m, k, \omega) + \chi_\pi^0(m, k, \omega)$ with

$$\chi_i^0(m, k, \omega) = \frac{n_i^0\left(k^2 + \frac{m^2}{R^2}\right)}{\beta\left(k^2 + \frac{m^2}{R^2}\right)^2 + \alpha_i\left(k^2 + \frac{m^2}{R^2}\right) - \omega^2 - i\gamma_i\omega}. \tag{6}$$

The external perturbing potential Φ_{ext} and the induced potential Φ_{ind} may be expressed as:

$$\Phi_{ext}(\rho, \varphi, z, t) = \int\frac{\rho_{ext}(\vec{r}', t)}{|\vec{r} - \vec{r}'|}d^3\vec{r}', \tag{7}$$

$$\Phi_{ind}(\rho, \varphi, z, t) = \int\frac{\rho_{ind}\left(\vec{r}', t\right)}{|\vec{r} - \vec{r}'|}d^3\vec{r}', \tag{8}$$

where $\rho_{ext}(\vec{r}', t) = Q(1/\rho')\delta(\rho' - \rho_0)\delta(\varphi' - \varphi_0)\delta(z' - vt)$ is the charge density external to the electron gas, $\rho_{ind}(\vec{r}', t) = -n(\varphi', z', t)\delta(\rho' - R)$ is the charge density induced on the electron gas, and $d^3\vec{r}' = \rho' d\rho' d\varphi' dz'$.

Knowing that the Coulomb potential in cylindrical coordinates may be written as a FB transform [15,19]:

$$\frac{1}{|\vec{r} - \vec{r}'|} = \frac{1}{(2\pi)^2}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} e^{im(\varphi-\varphi') + ik(z-z')}g_{mk}(\rho, \rho')dk, \tag{9}$$

where $g_{mk}(\rho, \rho') = 4\pi I_m(|k|\rho_<)K_m(|k|\rho_>)$ with $\rho_< \equiv \min\{\rho, \rho'\}$ and $\rho_> \equiv \max\{\rho, \rho'\}$, while I_m and K_m are cylindrical Bessel functions of integer order m, it is easy to obtain the FB transforms of the external and induced potentials as follows:

$$\Phi_{ext}(\rho, m, k, \omega) = 2\pi Q g_{mk}(\rho, \rho_0)\delta(\omega - kv), \tag{10}$$

$$\Phi_{ind}(\rho, m, k, \omega) = -Rg_{mk}(\rho, R)n(m, k, \omega). \tag{11}$$

Substituting Eq. (5) into Eq. (11) and using Eq. (10) one obtains:

$$\Phi_{ind}(\rho, m, k, \omega) = -2\pi RQ g_{mk}(\rho, R)g_{mk}(R, \rho_0)\chi(m, k, \omega)\delta(\omega - kv), \tag{12}$$

where $g_{mk}(\rho, R) = 4\pi I_m(|k|\rho)K_m(|k|R)$, $g_{mk}(R, \rho_0) = 4\pi I_m(|k|\rho_0)K_m(|k|R)$, and the density response function of a carbon nanotube is given by:

$$\chi(m, k, \omega) = \frac{\chi_0(m, k, \omega)}{1 + Rg_{mk}(R, R)\chi_0(m, k, \omega)}. \tag{13}$$

Finally, using Eqs. (4) and (12) one can obtain an expression for the induced potential as follows:

$$\Phi_{ind}(\rho, \varphi, z, t) = -4RQ\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} e^{im\varphi + ik(z-vt)}I_m(|k|\rho)I_m(|k|\rho_0) \times K_m^2(|k|R)\chi(m, k, kv)dk. \tag{14}$$

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

$$U_{im} = \frac{Q}{2}\Phi_{ind}(\rho, \varphi, z, t)|_{\rho=\rho_0, \varphi=\varphi_0, z=vt}. \tag{15}$$

Substituting Eq. (14) into Eq. (15) and setting $\varphi_0 = 0$, it is easy to obtain the following relation for the image potential:

$$U_{im}(\rho_0) = -4Q^2R\sum_{m=-\infty}^{\infty}\int_0^{\infty} I_m^2(k\rho_0)K_m^2(kR)\mathrm{Re}[\chi(m, k, kv)]dk, \tag{16}$$