Energy dependence of ion guiding through nanocapillaries

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Abstract. We present first simulation results for the energy dependence of the effective
guiding of ions through nanocapillaries in insulating materials based on classical transport
theory. We also investigate the dependence of guiding on the effective dielectric shielding near
the insulating surface. We find agreement with experimental data over a range of energies
without any freely adjustable parameter.

1. Introduction
The surprising discovery of guided transmission of highly charged ions (HCI) in their initial
charge state through insulating nanocapillaries [1] has stimulated a large number of investigations
employing various geometries and materials (e.g. [1-8]). Recently a guiding effect was found even
for electrons with an energy of several hundred eV [9, 10]. While the mechanism for the latter
is still unclear, for ion guiding the following scenario has emerged: during the charge-up phase,
projectiles with charge state \( q^+ \) entering the capillary under an angle of incidence \( \theta \)
larger than the geometric opening angle hit the capillary wall and deposit their charge. These charges
are transported along the surface and into the bulk of the target material. Projectiles entering
the capillary subsequently will be deflected due to the Coulomb field of the deposited charges
and may eventually be transmitted (see Fig. 1). Guiding (stable transmission conditions) sets
in as soon as a dynamical equilibrium between projectiles hitting the capillary wall (charging)
and transport into the bulk or to the capillary exits (discharging) has been established.

A theoretical description and \textit{ab initio} simulation of this process poses a considerable challenge
in view of the widely disparate times scales simultaneously present in this problem [11]. We
have therefore developed a mean-field classical transport theory [11] based on a microscopic
classical-trajectory Monte Carlo simulation for the ion transported, self-consistently coupled to
the charge-up of and charge transport at the internal capillary walls. The underlying idea is to
relate the microscopic ion-surface scattering and ion transport to known macroscopic properties
of the materials involved such as surface and bulk conductivity and the dielectric constant.
This allows to be predictive and for a description of the ion guiding without resorting to freely
adjustable parameters or additional ad-hoc assumptions. In the present communication we focus
on the energy dependence of guiding, for which experimental data have recently become available
[2]. We model transmission of Ne\textsuperscript{7+} ions with kinetic energies ranging from 2 to 9 keV through
PET nanocapillaries with a diameter of 200 nm (see schematic view in Fig. 1). The incident current was kept constant at a typical experimental value of 1 nA [1, 2]. Furthermore, we illustrate the importance of a proper description of dielectric shielding of the charges deposited on the surface.

2. Mean-field classical transport theory

We first briefly review the mean-field classical transport theory [11] employed in the present simulation. A projectile of charge state $q^+$ enters a capillary under an angle of incidence $\theta_{in}$ and with kinetic energy $E$. It travels within the capillary under the influence of the Coulomb field $V_C$ of partially screened charges on the capillary wall deposited earlier until it either leaves the capillary, i.e. to contribute to transmission, or collides with the interior wall of the capillary (i.e. contributes to beam loss). In the latter case, it neutralizes on a (sub-)fs time scale and deposits $q$ at charges at the surface. Charges deposited may diffuse along the surface or into the bulk. These processes are governed by their diffusion constants $D_s$ and $D_b$ which can be derived from material properties [12]. Motion of surface charges is modeled by an random walk which may eventually end with transport to the metal cover of the capillary target. When diffusing into the bulk, decay of charge carriers is characterized by a time-constant $\tau_b$ which is inversely proportional to $D_b$ [11]. Both bulk and surface diffusion are assumed to be independent of the charge density at the surface, i.e. charge transport is treated within linear response. Non-linear charge transport as recently suggested [3] is neither invoked nor necessary.

Within the framework of linear response, the bare charge $q$ deposited by the ion is screened by the dielectric medium. As the deposition occurs at the interface to vacuum, proper treatment of dielectric screening is required [13]. Denoting the bare Coulomb interaction between the guided ion and the charge deposited by $V_C$ the effective screened interaction, denoted by $V_{SCR}$, depends on the location of the deposited charge $q$. In the limiting case that the charge has already diffused into the bulk, bulk screening would apply, i.e. $V_{SCR} = V_C/\varepsilon$. We use here and in the following the static limit $\varepsilon = \varepsilon(q \to 0, \omega \to 0)$ of the dielectric function since the characteristic time for build-up of screening (time interval $\Delta t$ between two subsequent ions entering the capillary $\approx 10^{-10}$ sec) is very large compared to the characteristic time for optical excitations, $\Delta t \gg 2\pi/\omega_{opt}$. The dielectric screening of surface charges, is determined by the induced polarization, “image charge” [13] $\chi = (\varepsilon - 1)/(\varepsilon + 1)$. The effective residual charge and hence the effective potential is given by $V_{SCR} = V_C(1 - \chi) = 2V_C/(\varepsilon + 1)$. Our simulation employs the latter expression if not otherwise stated. To illustrate the significance of dielectric screening we will also show results using bulk screening instead as well as for bare interactions ($V_{SCR} = V_C$). Trajectories of guided projectiles are, in addition to the charge-up within individual capillaries, also affected by the mesoscopic fields of nearby capillaries. The latter predicts a dependence of the angular distribution on the mean-distance between capillaries or, equivalently the capillary density, an example of which will be shown below.
3. Results

Figure 2 presents total transmission in equilibrium as a function of θ_{in} for a projectile energy of \( E = 3 \) keV and \( E = 7 \) keV. Following Hellhammer et al. [14] total transmission of HCI through nanocapillaries is fitted by a Gaussian \( T(\theta_{in}) = T(0°) \exp(-\sin^2 \theta / \sin^2 \theta_g) \). Hence, transmission can be given in terms of the guiding parameter (“guiding power”) \( b = \sin^{-2} \theta_g \), or the effective guiding angle \( \theta_g \). At the guiding angle the transmission function has decreased to \( T(0°)/e \). The original motivation for the Gaussian ansatz was a Boltzmann type “thermalization” argument for the transverse energy. Note, however, that also other choices of fitting curves to \( T(\theta_{in}) \) perform similarly well. An example is shown for a square-Lorentzian in Fig. 2. By assuming guiding to be a statistical process, Refs. [2, 14] predict linear behavior for \( b \) as a function of \( E/q \). Fig. 3 shows the guiding parameter \( b \) as a function of the scaled kinetic energy \( E/q \). For comparison we show also simulation results assuming bulk screening as well as no screening at all (\( V_{SCR} = V_C \)). As expected, simulations invoking surface screening perform superior in reproducing the experimental data, the agreement is satisfactory. It should be noted that the approximately linear increase of \( b \) indicated by Fig. 3 cannot continue for higher \( E \). Instead, for large energies, \( b \) approaches a constant as soon as guiding breaks down and \( \theta_g \) becomes equal.
to the geometric opening angle. This saturation regime is not yet reached for $E/q \approx 1.5$ keV.

Another quantity of interest is the angular width $\Delta \theta_{\text{out}}$ (FWHM) of the guided beam upon exit. As transmission through a capillary with a geometric opening angle of $\theta_0 \approx 1^\circ$ should lead to a very narrow angular distribution, large values for $\Delta \theta_{\text{out}}$ observed in experiments (up to $5^\circ$) have been surprising and have created considerable interest as to its underlying mechanism. Trajectory simulations for a single capillary do not feature such broad distributions but show a width close to $\theta_0$. In previous work we have suggested the collective field created by charge patches of the ensemble of all capillaries illuminated by the primary beam to be a possible source of enlarged angular width [11]. It acts as an einzells in the exit region of the capillary deflecting projectiles close to the exit plane. Adding the influence of the resulting macroscopic field in our calculation leads to an energy dependence similar to the one observed in experiment (Fig. 4). The field strength is determined from the principal charge patch in the entrance region; the capillary density $N$ is assumed to be $N = 4 \times 10^8$ cm$^{-2}$. The dependence of $\Delta \theta_{\text{out}}$ on the scaled energy $E/q$ can be well fitted by $\sin^2(\Delta \theta_{\text{out}}) \propto (E/q)^{-1}$ in agreement with experimental data [2]. Such a collective effect immediately implies that $\Delta \theta_{\text{out}}$ should depend on the density of the capillaries, or equivalently, on the mean spacing between them. In particular, drastic reduction in capillary density should reduce $\Delta \theta_{\text{out}}$ to close to the geometric opening angle. Indeed, samples with significantly lower capillary density ($N = 4 \times 10^6$ cm$^{-2}$) show angular widths close to simulation results for a single capillary (see Fig. 4).

4. Conclusion

We have simulated ion transmission through insulating nanocapillaries using a mean-field classical-transport theory. Ion trajectories are propagated in the combined fields of charges deposited on the capillary wall, their polarization charges, the projectile image charge, and the macroscopic field from neighboring capillaries. The simulation avoids any freely adjustable parameters in order to be predictive and to provide qualitative insights into underlying mechanisms. We have varied projectile energy and angle of incidence and have tested different models of dielectric shielding. Best agreement with experimental data is found for dielectrically screened surfaces charges. Reasonable agreement with data could be found employing only macroscopic material parameters of PET like dielectric constant, surface and bulk conductivity.

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