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Simulation of guiding of highly charged projectiles through insulating nanocapillaries

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Abstract

Recent experiments have demonstrated that highly charged ions are guided through insulating nanocapillaries along the direction of the capillary axis for a surprisingly wide range of injection angles. Even more surprisingly, the transmitted particles remain predominantly in their initial charge state. We present a first theoretical treatment of ion guiding. We simulate the self-organized charge-up. Both the linear and non-linear response of the insulator surface to the local field are considered and partial agreement with experiment is found.

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Keywords: Ion-surface interaction; Ion-surface scattering; Ion guiding; Nanocapillaries

1. Introduction

The transmission of multiply and highly charged ions (HCI) through nano-capillaries has recently been used as a tool to study the interaction with surfaces, specifically, the internal wall of the capillary. The original motivation was to delineate the initial state of hollow-atom formation at large distance from the surface [1–3], information hardly accessible by scattering at flat surfaces. Image attraction and close collisions tend to erase the memory on this early state of ion–surface interaction when the ion suffers close encounter as it is either reflected from the topmost layer of the surface or penetrates into the bulk. As the ion can escape the capillary prior to a close encounter with the surface, the hollow atom can be directly spectroscopically accessed [1,4]. Initial investigations focused on metallic capillaries. Capillaries typically have a radius of $r = 50$–100 nm (“nanocapillaries”) and a length of 1 to 10 μm, thus featuring an aspect

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ratio of 1:10 to 1:100 and a geometric opening angle down to $\theta_0 < 1°$ (see Fig. 1).

Very recently, insulating capillaries made of track-etched polymers ("mylar") [5] and SiO_2 [6] have been used. Their transmission showed several surprising features. Most remarkably, ions retaining their *initial* charge state are transmitted even for injection angles θ_{in} much larger that the geometric opening angle θ_0 with θ_{in} up to 25°. Moreover, the angular distribution is found to be centered about the capillary axis with a spread (FWHM) of $\Delta\theta_{out} \approx 5°$ for mylar [5] but close to geometric opening θ_0 for SiO_2 [6]. Keeping the initial charge state, contrary to the expected neutralization upon approach of the internal capillary surface, suggests that the ions bounce off the walls at distances larger than the critical distance $R_c \approx \sqrt{2Q}/W$ [2] (Q: charge state; W: workfunction of capillary material). Key to this process is the charging up of the internal insulator walls due to ion impact. Ion guiding through the capillary ensues as soon as a dynamical equilibrium of self-organized charge up by the ion beam, charge relaxation, and reflection is established.

Simulation of this process is hampered by wide disparity of underlying time scales. While the local microscopic charge-up caused by an individual ion impact happens on a sub fs to fs scale, the mean time interval between subsequent ion impacts within the same capillary for typical beam current densities of nA/mm^2 is of the order of tens of ms. Dynamical equilibrium for guiding is only established after a few minutes i.e. (10^2 s). Finally, breakdown of the guiding condition due to discharging of the insulator walls is observed on the time scale larger than $\tau_d \gtrsim 10^3$ s [5,7,8]. In the following first attempt to simulate this complex process we focus on the microscopic build-up of guiding condition while treating the macroscopic discharging time τ_d due to current flow to the grounded metallic surfaces (Fig. 1) as a phenomenological free parameter. We simulate an ensemble of ions transported through an individual capillary randomly spaced in time with an average interval $\overline{\Delta t}$. The importance of collective effects such as intercapillary interaction and mesoscopic electric field emanating from the illuminating entrance surface will be discussed below. We find partial agreement with experimental data. We conclude this paper by pointing to future experimental and theoretical challenges to be overcome.

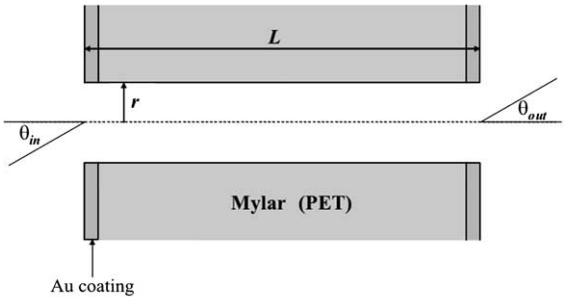

Fig. 1. Geometry of nanocapillary of length L and radius r. Ions enter at an angle θ_{in} and exit at an angle θ_{out} relative to the capillary axis.

2. Method of simulation

Consider the impact of a beam of ≈nA/mm^2 Ne^{7+} with total energies of a few keV on the entrance surface of the target 4% of which are covered by capillary openings and a beam spot size of about 1 mm^2. The average time interval between two projectiles entering the same capillary is $\overline{\Delta t} \gtrsim 10$ ms. The transit time of the ion through the capillary with a length of $L \cong 1$–10 μm is approximately 10^{-11} s, i.e. about 10 orders of magnitude shorter. Accordingly, calculation of the ion trajectory through a capillary is strictly a single-particle problem, however controlled by strong memory effects on previous impact events and, in turn, causing modifications of the internal electrostatic potential for subsequent trajectories.

Initially, ions entering with angles relative to the capillary axis larger than θ_0 will hit the internal wall depositing ($q + \gamma$) unit charges. A preliminary measurement of the secondary electron emission coefficient γ for Ne^{7+} striking a planar mylar surface found small values of $\gamma < 1$ [9]. Additional charge-up by secondary electron emission is therefore neglected in the following. Charge-up by electron emission may, however, be important for other surfaces. The initially localized charge will rapidly migrate by hole hopping. As no quantitative information on this process is known for