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Simulation of heavy-ion guiding in insulators

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Abstract

Guiding of charged particles through insulating target structures (capillaries, glass cones, parallel glass plates) has become a topic of considerable interest. It has been shown for insulating capillary targets that highly charged ions are deflected along the capillary axis while remaining in their initial charge state. Similar results have been reported for the focusing of ion beams by glass cones. We have developed a classical transport theory relating microscopic charge-up with macroscopic material properties. For insulating capillary transmission good agreement with experiments is found. Currently investigated experimental systems will be accessible to theory within the same framework.
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1. Introduction

The study of multiply-charged ion–solid interactions is of considerable technological importance for the understanding of material damage, surface modification, and plasma-wall interactions. Theoretical interest in the field is derived from the complex many-body response of surface electrons to the strong Coulomb perturbation. For insulating materials the question of charge transport within the target material opens an important side aspect of the interaction. It was speculated that local charge-up due to the transfer of electrons from the surface to the projectile would lead to backscattering of still positively charged projectiles (''Trampoline effect'' [1]), however, direct evidence for this process was not found so far. Theoretical studies showed [2] that charge transfer within insulators is in most cases fast enough to prevent backscattering from the self-induced depletion charge.

Another process connected to local charge-up of an insulator surface is the deflection of incoming charged projectiles by the macroscopic charge patch formed by other ions hitting the surface in earlier stages of the experiment. This effect was used lately to deflect ions along the axis of capillary targets made of insulators (PET [3,4], SiO_2 [5]). Similar experimental geometries are also investigated in Vienna [6] and Tokyo [7]. Meanwhile, also other experimental geometries (glass cones [8], parallel glass plates [9]) are under investigation.

Key to the understanding of these experimental findings is the notion of the two distinctly different time constants for charge transport along the surface and within the bulk of insulators. The interplay between these time constants is responsible for the formation of a dynamic equilibrium keeping up a Coulomb field large enough to deflect charged particles and small enough not to cause a Coulomb blockade of the entrance to the micro- or nanostructure [10]. We test our model for the transport of charged particles through insulating capillaries. Experimental conditions [3,5] are idealized the following way (see Fig. 1): the array of nanocapillaries is represented by a single cylindrically shaped canal through the material with given dielectric constant ε and surface and bulk conductivities σ_s and σ_b. The influence of charge-up in other capillaries on the potential deflecting the projectile trajectory is taken into

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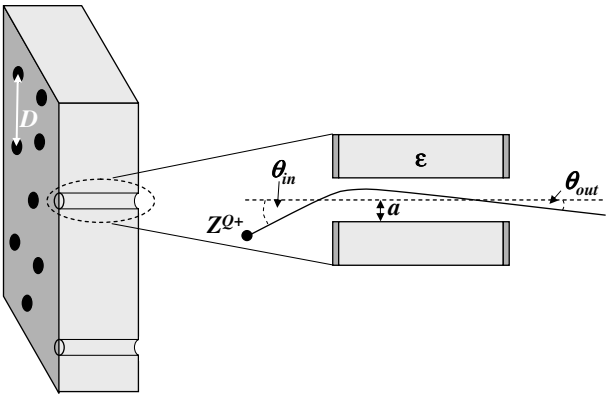

Fig. 1. Ion-nanocapillary interaction, schematically: an array of nanocapillaries is oriented along the surface normal. Transmission through an individual capillary is simulated. The insulating material with dielectric constant ε is covered on both sides with gold layers (dark shaded). We model capillaries with a typical diameter $d = 100$ nm and length $L = 10$ μm.

account as an averaged condenser field (see Section 2.2). We compare our predictions with recent experimental data [3,5–7]. An outlook to simulations for other experimental geometries will be given at the end of this contribution.

2. Simulation method

Simulation of ion guiding through insulating structures has to bridge widely disparate time scales immanent to this problem [10]:

- The microscopic charge hopping along the surface after impact of projectile ions takes place on a sub-fs to fs scale.
- Depending on the ion energy the transmission time τ_t of a projectile ion through the capillary can become as large as $\tau_t \approx 10^{-10}$ s.
- In capillary experiments, typical time intervals $\overline{\Delta t}$ between two subsequent transmission (or impact) events in the same capillary are, for present experimental current densities of nA/mm^2 of the order of $\overline{\Delta t} \approx 0.1$ s.
- Characteristic (bulk) discharge times τ_b (related to the bulk-hopping time) can be estimated from the measured conductivity of the target material and can even reach days.

It is evident, that no fully microscopic ab-initio simulation can cover these 18 orders of magnitude. Macroscopic parameters such as the hopping time deduced from material conductivities are therefore included as an external, but not freely adjustable parameter to a classical transport simulation for the interaction of the projectile with the target and its Coulomb field. The present approach is therefore a mean-field classical transport theory (CTT, [11]) based on a microscopic classical-trajectory Monte Carlo (CTMC) simulation for the ion transport. Dynamic equilibrium is established by the self-consistent coupling of the ion transport to the charge-up of and charge diffusion near the insulating surfaces.

2.1. Projectile trajectories

Projectile transport is simulated by solving Hamilton's equation of motion

$$\dot{\vec{R}} = \frac{\partial H}{\partial \vec{P}} \quad \dot{\vec{P}} = -\frac{\partial V}{\partial \vec{R}}. \tag{1}$$

The incidence angle θ_{in} is chosen from a Gaussian distribution around the nominal entrance angle with a full width at half maximum of $\Delta\theta = 0.5°$, the initial lateral position from a uniform distribution over the capillary entrance. The trajectory calculation is started at a distance of 10 000 a.u. (500 nm) from the target surface, i.e. before entering the capillary. Memory effects are built into the potential V (Eq. (1)) by following the charges deposited on the surface or diffused into the bulk of the target material (see Section 2.2). The trajectory therefore depends on the history of previous trajectories through the same capillary and is additionally influenced by the mean field of neighboring capillaries.

In order to save computing time, we have developed an algorithm that solves Eq. (1) approximately while retaining the accuracy of ordinary differential-equation solvers. To this end, we have divided the capillary into tetrahedrons for which we calculate an approximate constant electric field from the potential at the corners. Propagation within a tetrahedron can then be solved analytically reducing a full simulation of the trajectory to a sequence of calculations of entrance and exit points into and out of individual tetrahedrons. Comparison of our method and a fourth-order Runge–Kutta simulation is used to determine the optimal size of the tetrahedrons.

The propagation of the trajectory is stopped if either the projectile reaches the capillary exit or hits the surface. The point of impact serves as starting point of the simultaneously performed calculation of the charge diffusion. Between subsequent trajectories diffusion of surface charges is determined for the time interval Δt between two subsequent trajectories.

2.2. Potentials

In our model the updating of the effective potential proceeds as follows: prior to entering of an ion into the capillary, the force acting on the projectile is calculated from

$$\vec{F} = \vec{F}_{im} + \vec{F}_{wall} + \vec{F}_{mean}, \tag{2}$$

where F_{im}, F_{wall}, and F_{mean} describe the interaction of the ion with its own image field, the combined fields of charges deposited on the internal capillary wall by earlier projectile impacts, and the mean field exerted by all other capillaries of the target, respectively. F_{im} can be calculated from

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