Interaction of slow highly charged ions with solid surfaces

J. Burgdörfer, C. Lemell, C. Reinhold, K. Schiessl, B. Solleder, K. Tökesi

Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraβe 8-10, A-1040 Vienna, Austria

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. The recent availability of sources for slow highly charged ions (HCl), namely electron cyclotron resonance (ECR) and electron beam ion sources (EBIS) has led to a flurry of research activities, both experimental and theoretical, in the field of HCl-solid interactions [1-3]. On the most fundamental level, its importance is derived from the complex many-body response of surface electrons to the strong Coulomb perturbation.

Due to the intrinsic multi-particle nature of the interactions large systems have to be simulated requiring the use of large scale computer systems. Depending on the type of simulation (Classical Trajectory Monte-Carlo (CTMC) simulation, ab-initio density-functional theory (DFT), time-dependent DFT) we use different types of computers optimized for serial processing (CTMC – low memory requirements, high clock rate) or linear algebra (DFT – large memory, broad and fast data bus). As an example we present in this report results for the transmission of highly charged projectiles through capillary targets.

During the recent year we have performed a broad range of simulations to study the interaction of HCl with capillary surfaces in detail. In particular, we have concentrated on the simulation on projectiles which did not change their initial charge state during the interaction (trajectories of type (3) in Fig. 1).

Figure 1: Schematic picture of a capillary and three types of trajectories.

During the recent year we have performed a broad range of simulations to study the interaction of HCl with capillary surfaces in detail. In particular, we have concentrated on the simulation on projectiles which did not change their initial charge state during the interaction (trajectories of type (3) in Fig. 1).
Transmission of HCI through insulating capillaries

Very recently, capillaries through insulating foils (PET ("Mylar") [5] and SiO$_2$ [6]) have become available. Unexpectedly, considerable transmission rates for projectiles in their initial charge state were measured for incidence angles as large as $25^\circ$. Interpretation of these results run along the following lines: First, projectiles hitting the capillary surface close to its entrance area deposit their charge at the surface which - due to the small conductivity of the material - remains localized in a self-organized charge patch. Projectiles entering the capillary in a later stage of the experiment are detected by the Coulomb field of the charge patch passing the surface in a distance larger than the critical distance for charge transfer $R_c \approx \sqrt{2Q/W}$ as predicted by the classical over barrier model [2] with $Q$ and $W$ being the projectile charge state and workfunction of the capillary material, respectively.

Our simulation consists of several ingredients bridging processes occurring at vastly different time scales: form microscopic charge-up ($\sim 10^{-15}$ s), to transport of a single ion ($\sim 10^{-10}$ s) through the capillary, to the approach of dynamical equilibrium ($\sim 10^2$ s). Ion trajectories are started well outside the metallic layer covering the insulator and end either with the transmission through the exit opening of the capillary or with the impact on the capillary surface. In the latter case $Q$ charges are deposited on the surface where $Q$ is the initial charge state of the projectile. Due to the finite conductivity of the target material these charges move along the capillary wall or, with a small probability, diffuse into the bulk. Projectile trajectories are calculated taking into account the electric field of charges deposited previously on the capillary wall. We were able to reproduce the transmission rates for HCI transmitted through Mylar and SiO$_2$ capillaries at energies ranging from 3 keV to 7 keV.

Consistent with experimental findings we observe increasing differences in the angular distributions of transmitted ions parallel and perpendicular to the plane of incidence with increasing $\theta_{in}$. In Fig. 2 we show the two dimensional distribution of exit angles for $\theta_{in} = 0^\circ, 1^\circ, 3^\circ$, and $5^\circ$. The distribution normal to the plane of incidence ($\gamma$-direction) remains almost constant for all angles. Parallel to the plane of incidence a slight widening and displacement of the peak from the center of the distribution is found. This is in agreement with experiments showing a small deviation of the centroid of the scattering.
distribution towards larger deflection angles.

References


