B.4.1. Charge Exchange in Ion-Surface Collisions—*U. Thumm*

We investigated charge exchange and hybridization for slow protons, He^{+}, Li^{++}, and Be^{3+}, and highly charged ions interacting with metal and insulator surfaces, including effects of external electric fields (Publication #85).

B.4.1.1. Close-Coupling Calculations for Non-Penetrating Ion-Surface Collision

We continued to develop our two-center close-coupling code [1] for charge exchange and resonance formation in ion-surface interactions. In this approach, the dynamics of the active electron in the Hilbert space spanned by the metal orbitals is reduced to a self-energy term, which involves a pole approximation, and which acts as a complex optical potential in the subspace spanned by the projectile orbitals.

In order to resolve the dynamics in the subspace spanned by the metal orbitals, we started to develop a new method, in which the continuum of metal conduction band states is explicitly taken into account. This is achieved by solving the time-dependent Schrödinger equation for the active electron interacting with the slow projectile and a metal surface within a basis of hydrogenic projectile states (in parabolic representation) and discretized conduction band states (Publication #92, Accepted Publication #1). Our results show the evolution of projectile and substrate population amplitudes and allow for the distinction of qualitatively different interactions regimes: while at larger particle-surface distances Stark-like hybridization without charge exchange prevails, the charge transfer starts at smaller distances, where the hybridization pattern cannot be described in terms of Stark states.

B.4.1.2. Influence of Static External Electric Fields on Charge Exchange and Resonance Formation

We investigated the ionization of Rydberg atoms in front of a metal surface under the influence of an external electric field (Publication #29). Focusing on low energy collisions, we used the adiabatic self energy method [1] to generate resonance states formed during the interaction of an ion with the surface, together with their adiabatic energy shifts and widths, over a wide range of ion-surface distances. The corresponding adiabatic ionic hybrid states served as a convenient and physically motivated set of basis functions for our time-dependent close-coupling calculation. This calculation allowed us to investigate the time evolution of the net projectile charge as a function of various parameters, such as the initial projectile charge, the projectile velocity, and the strength of an applied external field.

B.4.1.3. Extended ab-initio Close-Coupling Calculations for Bare Incident Ions Interacting with Metal Surfaces

Within our two-center close-coupling approach, we investigated the hybridization of He^{++}, Li^{3+}, and Be^{4+} ionic levels and the formation of surface resonances induced by interactions with an Aℓ surface (Publication #32). We obtained converged results for resonance energies, widths, and electronic density profiles for resonances that for large ion-surface distances merge into hydrogenic states with principal quantum numbers $n < 8$.

B.4.1.4. Interactions of Ions with Thin Metallic Films

We studied the broadening of atomic levels near thin metallic films within the fixed-atom approximation. We calculated first-order level widths by using a Jennings-type jellium potential to describe the electronic states of the film, and hydrogenic wave functions in parabolic (Stark) representation for the atomic orbitals (Publication #87). In the parabolic representation, hybridization effects due to the long-range image-charge interactions were taken into account. Size quantization in the growth direction of the film was found to give rise to characteristic structures in the level widths, atomic occupation probabilities, and transition distances as a function of the film thickness. Details of these structures depend on the orientation of the Stark orbitals with respect to the film and were traced to the dependence of transition matrix elements on the active electron's wave vector component parallel to the surface for the case of a semi-infinite metal. The extremely large variation of the calculated transition distances with the film thickness may result in observable effects in atomic interactions with thin films.

B.4.1.5. Classical Over-Barrier Simulations for Highly Charged Ions Interacting with Metal and Insulator Surfaces

The classical over-barrier simulation for slow highly charged ion — surface interactions has been very successful for the case of metal surfaces [2]. We have written a new and extended classical over-barrier code, which applies to metal and insulating (ionic crystal) surfaces and found good agreement of our simulated projectile energy gains with experiments on LiF and KI surfaces (Publication #26) (within large experimental error bars). As insulator specific effects, we included local charge accumulations and work function changes at the surface.

B.4.1.6. Classical Over-Barrier Simulations Including Side-Feeding Processes

We have investigated the neutralization and relaxation dynamics of slow multiply charged ions during their interaction with metal and insulator surfaces within an extended over-barrier model. Our approach includes a Monte Carlo sampling over projectile trajectories and elementary electronic processes in combination with the online computation of Auger rates and projectile energy levels within a standard atomic structure code (Publications #79 and 108). Special emphasis was devoted to near-surface interaction mechanisms. Sampling over full projectile trajectories and incorporating atomic structure calculations, we simultaneously obtained projectile energy gains, final charge state distributions, and Auger electron yields, all in reasonable agreement with recent experiments. With respect to insulator surfaces, we have addressed the influence of insulator-specific effects, such as the capture-induced accumulation of localized surface charges and work function changes, on the projectile trajectory, population dynamics, and final charge state of the projectile (Publications #79 and 108). Including these effects, we computed projectile kinetic energy gains that agree with experimental data.

References

1. P. Kürpick, U. Thumm, and U. Wille, Nucl. Instrum. Methods B 126, 273 (1997); P. Kürpick, U. Thumm, and U. Wille, Phys. Rev. A 56, 543 (1997).
2. J. Burgdoerfer, C. Reinhold, and F.W. Meyer, Nucl. Instrum. Methods B 98, 415 (1995).