

NEUTRALIZATION OF H^- ON Cu SURFACES: LIFETIME VERSUS TRAJECTORY

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The resonant charge transfer (RCT) phenomenon of atomic anions interacting with surfaces is important in many fields of physics and technology, namely, surface chemistry, secondary anion mass spectroscopy, particle detection, and plasma wall interactions. It, thus, becomes of practical importance to study the relative role of different dynamical aspects, such as, the lifetime of populated metallic states and the projectile trajectory, in influencing the process.

We consider an H^- ion *specularly* scattered from Cu surfaces of the symmetries (100) and (111), each having a band gap in the direction normal to the surface with $Cu(111)$ holding a surface state inside the gap. The ion is described in an open shell single active electron model[1]. A one dimensional effective potential, constructed from pseudopotential local density calculations, is employed to model the surface[2]. The ion moves in a classical trajectory obtained via a plane-averaged interatomic potential[3]. We employ the Crank-Nicholson propagation over a two-dimensional grid, in which the continuum is approximated by adding the free motion in a direction parallel to the surface.

With increasing angle of incidence Θ (decreasing ion-surface interaction time as well as distance of closest approach D_{close}), we find dramatically higher ion survival for collisions with $Cu(111)$ than with $Cu(100)$ (see Fig.1). For $Cu(100)$, where the ion interacts with the metal valence band directly, the survival probability tends to saturate around $\Theta=60^\circ$, beyond which the difference in trajectories is practically irrelevant. The steeply rising survival with higher Θ for $Cu(111)$, on the other hand, is a result of the capture in the localized surface state as well as the *transient* appearance of ion-induced laterally confined hybrid states that increasingly resists the electronic decay as D_{close} decreases.

With decreasing Θ , V_{nor} reduces resulting in longer interaction times, allowing all surface-localized states to decay while being simultaneously re-populated by the ion. Thus, going down

in Θ , the difference between ion-survival probability for $Cu(111)$ and $Cu(100)$ decreases. Moving below $\Theta=20^\circ$, however, the ion survival from either surface rises and becomes almost equal at 10° . This is because the increase of D_{close} progressively reduces the charge transfer rate such that any surface structural difference becomes largely irrelevant.

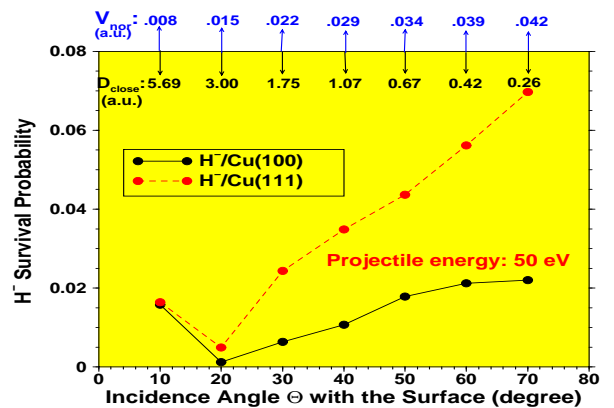


Fig. 1. H^- survival probability versus incidence angle Θ . Ion normal velocity V_{nor} and D_{close} are shown along upper x -axis.

Our results show that the projectile trajectory and the decay widths of ion-populated metallic as well as hybrid states crucially control the RCT process. This work is supported by the NSF (grant PHY-0071035) and the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, US DoE.

References

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