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Charge-transfer dynamics in anion collisions with vicinal nanostepped surfaces

Charge-transfer dynamics in anion collisions with vicinal nanostepped surfaces

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Synopsis We investigate the electron dynamics at various monocrystalline metal surfaces with stepped vicinal nanostructures. The unoccupied bands of the surface superlattice are resonantly excited *via* the charge transfer interaction of the surface with a H^- ion which flies by at grazing angles. The ion survival exhibits modulations as a function of the vicinal-terrace size and shows peaks at energies that access the image state subbands.

Vicinal surfaces of regular arrays of linear steps, prepared by cutting and polishing a single crystal by ultra-high vacuum methods, are the simplest models of lateral nanostructures on surface. These systems closely mimic rough industrial surfaces and are critical for their catalytic properties, without losing the lattice periodicity [1]. Thus, understanding electronic motions in these surfaces are valuable.

The charge transfer interaction dynamics of an ion with a surface is very sensitive to the surface band structure. The energy conserving transfer of an electron, the resonant charge transfer (RCT), occurs when the shift of the ion level enables the transfer to (from) an unoccupied (occupied) resonant state of the substrate. While studies on flat surfaces are aplenty [2], the first study on vicinally stepped Pd(111) is reported by us [3]. Calculations are now extended for other surfaces, such as, Cu(111) and Au(100) with vicinal steps, to probe important effects of superlattice dispersions.

We model the vicinal structure in a Kronig-Penny scheme. The RCT interactions of the H^- ion grazing the surface is simulated in a quantum mechanical wave packet propagation approach utilizing the split-operator Crank-Nicholson propagation method [3]. Thread based parallel computing using OpenMP was employed. Visualizations of the evolving wave packet density from the ion to the surface and back in the close interaction zone as well as its decay through the surface into the bulk *via* subbands of various surface specific states are made. Further, the survival probability of the ion is calculated as a function of ion's parallel velocity for varied sizes of the vicinal terrace.

The H^- survival probability are presented in Figure 1 showing strong modulations for stepped surfaces compared to the steady result of flat precursor surface. When the ion's parallel energy parabolic dispersion matches an image subband state, a resonance-type condition is reached, and, consequently, the recapture rate by the ion increases. This effect produces peaks in the survival probability as seen which appear largely insentive to the ion's strike location.

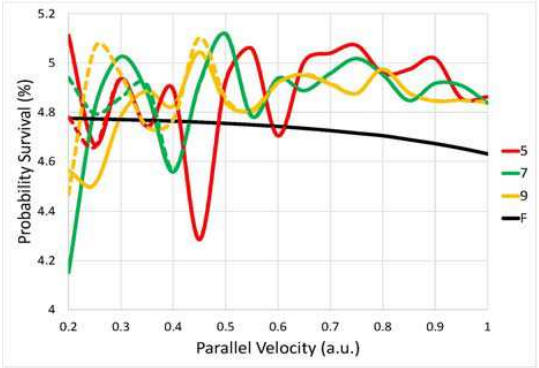

Figure 1. Ion survival for flat (F) and stepped Cu(111) as the ion strikes the center (solid) and step (dashed) of the terrace of sizes in units of lattice spacing.

The work serves as the proof-of-principle in the utility of our computational method to address surfaces with nanometric patterns.

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References

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