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Energy shift of He groundstate close to an aluminum surface

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Abstract

He atoms and ions with keV energies are scattered under a grazing angle of incidence from a flat and clean Al(1 1 1) surface. From the analysis of angular distributions for scattered projectiles we reveal that the angular shifts between distributions for incident neutral atoms and positive ions show a reversal in sign as function of distance of closest approach to the surface plane. This observation allows us to deduce the energy shift of the He groundstate as function of distance from the surface. Our work provides important information towards a fundamental microscopic understanding of atomic interactions close to metal surfaces.

Keywords: Charge exchange; Ion surface scattering; Noble gas ions; Metal surface; Helium; Aluminum; Level shift; Auger neutralization

Electronic interactions of atoms and ions with solid surfaces play an important role for a variety of processes and applications as, e.g., surface analytical tools, particle detection, or plasma wall interactions. A substantial amount of work in fundamental research can be found on investigations of the relevant microscopic mechanisms. These interaction mechanisms depend strongly on the kinematic regime of the collision with the target surface, characterized by projectile energy and collision geometry. Of considerable interest are collisions in the hyperthermal regime where projectiles do not penetrate the vacuum–solid interface. Then electronic interactions and charge transfer take place in front of the topmost layer of surface atoms, and atom–surface interactions can be studied under controlled conditions.

In this regime, two basic mechanisms are relevant for the neutralization of ions: (a) resonant neutralization (RN) where the energy of the electron active in charge transfer is conserved during the transition, and (b) Auger neutralization

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(AN), an inelastic tunnelling process where two electrons are involved in the transition. For atoms with high binding energies RN can be often neglected, i.e., for most combinations of noble gas atoms with metal surfaces, and AN will dominate charge transfer. Considerable progress has been achieved in recent years as to quantum mechanical treatments of the microscopic interactions.

The theoretical description of AN at surfaces is an intricate problem. This process takes place in the electron selvedge of the surface where screening effects and perturbations by the ion, affected by the broken symmetry at the interface, play an important role. Early quantum mechanical calculations gave AN transition rates [1] which were several orders of magnitude smaller than those derived from experimental data [2–4]. This discrepancy between theory and experiment, however, could not be removed by more recent and sophisticated calculations focusing on the model system He–Al (simple electronic structure, no contributions from RN [5]) [4–13].

The (modified) groundstate energy of the atom close to the surface plays a key role for a detailed understanding of atom–surface interactions. Until recently the shift of the binding energy of atoms close to a metal surface was approximated by the concept of classical image charges. Based on the pioneering work of Hagstrum [2] distances for charge transfer were derived from energy shifts in electron spectra resulting in AN transition rates, several orders of magnitude larger compared to theory [3,4]. A solution of this problem was recently proposed by van Someren et al. [12], Merino et al. [6], and More et al. [8]. In the latter theoretical studies, for AN of He^+ ions in front of an Al surface the description of the shift of the He groundstate energy by the classical image charge approach breaks down at several a.u. (atomic units) from the topmost layer of surface atoms as result of short-range chemical interactions. Two alternative scenarios were discussed [8,12,14]: (1) "high" transition rates (larger distances of neutralization) and validity of the concept of classical image charges for the description of level shifts, or (2) "low" transition rates (smaller distances of neutralization) and deviations from such a description of level shifts.

Evidence for scenario (2) was found by the survival of a small fraction of incoming ions in recent experiments on the neutralization of He^+ ions during grazing scattering from Ag and Cu surfaces [14–16]. In this regime of ion scattering (surface channeling [17,18]), this can only be understood by sufficiently small charge transfer rates.

As direct consequence of the small AN rates compared to RN, electron transfer proceeds relatively close to the surface. This allows one to study details of atom–surface interactions in a domain hardly explored so far. For a fundamental understanding of the interaction mechanisms, it is important to provide information on the energy shift of the groundstate of He atoms $\Delta E_{1s}(z)$ as function of distance z from an Al surface. In this work, we report on detailed studies to derive this quantity from scattering experiments with He atoms and ions using [5,8,10,18,19]

$$\begin{aligned}\Delta E_{1s}(z) &= E_{1s}(z) - E_{1s}(\infty) \\ &= V_{He^0}(z) - V_{He^+}(z)\end{aligned} \quad (1)$$

with E_{1s} being the binding energy of the He groundstate and V_{He^0}, V_{He^+} the scattering potential for He^0 atoms and He^+ ions, respectively. Our investigation was motivated by a recent experimental study on AN via electron spectroscopy by Lancaster et al. [20] which is interpreted in terms of an enhanced He binding energy close to the surface.

In the experiments we have scattered He^+ ions and He^0 atoms under a grazing angle of incidence Φ_{in} of 1–3° from a clean and flat Al(1 1 1) surface which was prepared by cycles of grazing sputtering with 25 keV Ar^+ ions and subsequent annealing. Projectiles are recorded at a distance of 66 cm behind the target by means of a position sensitive channelplate detector. Atoms and ions in the scattered beam are separated by a pair of electric field plates in order to measure charge fractions.

In Fig. 1 we show ion fractions after scattering of He^+ ions with energies ranging from 0.8 to 3 keV from Al(1 1 1) as function of normal energy $E_z = E\sin^2\Phi_{in}$, tuned by the adjustment of the incidence angle Φ_{in}. The small but defined fractions for impact of ions are attributed to a survival of projectiles in the initial charge state [14–16]. The