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$H^+$/Al(111) collisions

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Neutral fractions calculations for grazing incidence $^3$H/Al(111) collisions

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Synopsis We have calculated outgoing H(1s) fractions in a large range of impact velocities for protons impinging on Al(111) with a grazing incidence of 0.5°. Capture and loss for Resonant and Auger processes are taken into account and the role of the surface-plasmon-assisted electron capture mechanism is also investigated. Consideration of all these mechanisms allow to reach a good agreement with experimental measurements. A detailed analysis of our results show that Resonant processes dominate for $v_\parallel \leq 1.5$ although the surface-plasmon-assisted capture mechanism has a significant contribution around the Fermi velocity ($v_\parallel = 0.9$). For higher velocities Auger capture and loss mechanisms (and also Resonant loss) mainly explain the experimental findings.

It is well known that Resonant Capture (RC) and Resonant Loss (RL) processes play an important role in the $^3$H/Al reaction since the H ground state is always resonant with occupied levels of the metal. It has also been found that Auger Capture (AC) and Auger Loss (AL) mechanisms contribute significantly in particular for high impact velocities [1]. Furthermore, the surface-plasmon-assisted electron capture process (energetically forbidden at low velocities) exhibit transition rates whose magnitude is comparable to those of RC and AC mechanisms around the Fermi velocity [2].

In order to study the interplay of these processes for proton neutralization in grazing Al(111) surface scattering, dynamical calculations have been performed by means of the ETISc1D code [3] that allow to compute charge fractions and angular distribution of scattered species. We have used the dynamical image potential obtained in [4] while the purely repulsive potential is represented through the ZBL screening function. Since Resonant [5−7] and Auger [8] transition rates have been so far calculated in the static case, we use the method proposed in [9] to compute the corresponding velocity dependent Resonant and Auger rates. This approach based on the simplifying assumption that velocity dependent matrix elements are isotropic in the k-space, allow to factorize the velocity dependence of the rates in the so called “kinematic factors”.

We report in Fig. 1 a comparison between three calculations in which all the processes have been considered together with experimental neutral fractions [10] as functions of the ion velocity. In all cases the static Auger rates of [8], supplemented with the kinematic factors, are used as well as our results [2] for the surface-plasmon capture process: calculations I, II and III correspond (respectively) to the use of the H(1s) energy and the static resonant rates (also supplemented with the kinematic factors) of [5], [6] and [7]. These results reported in [5−7] present strong differences either quantitative for the magnitude of the rates or qualitative for the behavior of the H(1s) level near the surface. The differences between the three calculations of Fig. 1 at low and high velocities are mainly due to the sensitivity of both Resonant and Auger kinematic factors to the final atomic energy while the magnitude of the static rates play a minor role due to the capture-loss interplay. RC and RL mechanisms play the dominant role for $v_\parallel \leq 1.5$ whereas for higher velocities AC, AL (and also RL) processes mainly account for the experimental results. The effect of the surface-plasmon process is noticeable for 0.5°$\leq v_\parallel \leq 1.2$.

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