§17. Time-dependent Density Functional Study on Excited Hydrogen Atom Formation via Non-resonant Electron Capture by a Proton from Refractory Metal Surfaces

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Excited state abundance in neutrals reflected at refractory metals has been an issue of study concerning the plasma-wall interaction in nuclear fusion devices. Dα emission has been observed from the reflected neutrals of a deuteron beam at a molybdenum surface[1]. However, the mechanism of the excited state formation has been little understood. Excited levels of the atomic hydrogen are above the Fermi level of the molybdenum by a few eV. Surface electrons hardly transfer to such the shallow levels via tunneling or classical-over-the-barrier, unless some surface impurities decrease the effective work function substantially. The effect of the surface impurities has not been studied in the present work; we have investigated other (non-trivial) mechanism first[2].

In the present work, the non-resonant single-electron capture by an outgoing proton from metal surfaces was studied by means of the semi-classical theory (electronic transition was treated quantum mechanically, while proton motion was represented by classical trajectories). Early studies on the electron transfer have been undertaken with the aid of simplified interaction matrix elements and/or the adiabatic approximation, e. g. Brako and Newns[3] and Burgdörfer et al.[4]. The present study is based upon direct numerical solutions of the time-dependent Schrödinger equation including accurate interaction potentials.

Present calculations were performed for tungsten and molybdenum slabs whose widths are about 100 a. u. (about 5 nm). At low proton velocities, the occupation probability of the ground level (n=1) is almost unity, whereas those of the excited levels are vanishingly small as expected in the adiabatic approximation. As the velocity increases, the probabilities of the excited levels grow, while that of the ground level declines. A hump was found in the n=2 occupation probability at low velocities. It may be attributed to the oscillatory transition between quasi-resonant states of the n=2 level and a discrete conduction level of the metal slab. With the larger slab width (the higher number density of the conduction levels), the hump becomes less significant. For the semi-infinite metal, the hump should disappear after the transition amplitude is integrated over the continuous conduction band in which the atomic levels are embedded (bandwidth effect).

It is noted that the present model is based upon the dispersion relation of the quasi-free electron-gas. However, transition metals like tungsten have substantially different density of states from that of the free electron-gas. An improved model taking account of a correct density of states is under development. The Auger deexcitation might depopulate the excited levels, while it is left for future studies.

References

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