§8. Excited-State Abundance in Hydrogen Atoms Coming Out of Refractory Metal Surfaces


Electron transfer between hydrogen atoms and refractory metal surfaces was studied quantum mechanically [1]. The study is important to understand excited-state abundance in hydrogen atoms coming out of plasma facing walls.

Hα emission in boundary and divertor plasmas is a primitive probe for flux of the hydrogen atoms from the walls. The line-integrated Hα intensity along a perpendicular to the wall was estimated in the simple corona model. It was found that the intensity would depend strongly on the excited-state abundance in the hydrogen atoms coming out of the wall. However, the excited-state abundance is little understood. In this work, we investigated theoretically occupation probabilities for the excited levels of the atomic hydrogen after single-electron capture by a proton from the refractory metal surface like tungsten and molybdenum. To that end, it was necessary to develop quantum mechanical theories to describe energy structures (i.e. shift and broadening) of the hydrogen atoms placed near the metal surface and dynamic time-evolution of electronic states during the electron transfer process between the moving proton and the metal surface.

It is noted that the Auger neutralization (two-electron process) is expected to have minor contributions for the tungsten and molybdenum, since the ground level of the atomic hydrogen is resonant with the occupied conduction bands. The Auger de-excitation may also make some contributions to de-population of the excited levels of the atomic hydrogen. However, they are omitted in the present work.

The energy level structures were calculated using appropriate electron-metal surface interaction potentials. The interaction potentials include those of the surface-dipole layer, the exchange-correlation of conduction electrons, and the static dielectric response induced by the proton. The former two potentials were approximated by a semi-empirical formula established for modeling of LEED spectra [2]. The dielectric response was represented by a linear density response function obtained using the Kohn-Sham wavefunctions of the conduction electrons [3]. It was deduced from the calculated level structures that the n=3 excited state would hardly survive as far as about 15 Å distant from the tungsten surface.

The single-electron capture by the proton coming out of the tungsten surface was studied using a one-dimensional mixed quantum-classical method at the proton velocities of 0.1-1.0 a.u. The time-dependent Schrödinger equation of the electron was solved numerically using the split-operator spectral method [4], while the proton is assumed to move along a classical trajectory. At the lower velocities, the occupation probabilities of the excited levels were vanishingly small as expected in the conventional adiabatic theory. However, at the higher velocities (as high as the Fermi velocity of the metal), the occupation probability of the n=3 excited level reached to a few % of that of the ground level. This result is significant for the line-integrated Hα intensity: It is estimated that a few % rise in the excited-state abundance would increase the line-integrated Hα intensity to a few tens %, provided the ionizations per Hα photons are assumed to be about 10-20.

References