

## §22. Study on Excited State Distribution of Reflected Hydrogen Atoms at Metal First Walls by the Quantum-classical Mixed Model

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Excited state abundance in neutrals of proton reflected at metal surfaces has been an issue of study concerning hydrogen recycling diagnostics/modeling in magnetic fusion devices. It has been observed experimentally that population of the  $n=3$  levels of atomic hydrogen were created at metal surfaces for an incident proton beam with energy of a few keV or higher<sup>1)</sup>. It is obvious that the higher reflection coefficients at the surface, more abundant the excited atoms coming out of the surface provided the excited states were formed at the surface. However, the excited state formation is in question for lower energy protons backscattered at the surface.

In present works, the excited state formation was investigated in terms of electron transfer at the metal surface. A quantum-classical mixed model based upon semi-classical theories was used to evaluate occupation probabilities of atomic levels above the metal surface. In the semi-classical theory, electronic transition was treated quantum mechanically, while proton motion was represented by classical trajectories. Metal electrons were approximated by free electrons moving in a uniform positive charge distribution (jellium model), and the metal surface was represented by a jellium edge. Electrostatic interaction between a hydrogen atom and the surface electrons was approximated by linear density response taking correct Fermi energies and work functions of metals into account.

In one-dimensional model: Degrees of freedom were restricted to surface normal, calculations for occupation probabilities of the excited levels were performed for a proton receding from a tungsten surface at velocities of 0.1-1.0 a.u. (1 a.u.  $\approx 2 \times 10^6$  m/s). Mechanisms of the excited state formation were explained in terms of a Fermi sphere shifted by proton velocities relative to the surface<sup>2)</sup> and non-adiabatic promotion of electronic excitation<sup>3)</sup>. It was suggested that metals of higher atomic numbers would produce larger fraction of the excited states in neutrals from the surfaces due to higher energy reflection.

A three-dimensional model is being developed for more

accurate treatment of interaction and electron transfer between atoms and metal surfaces. The 3D model requires accurate electronic wave functions at each distance from the surface. A novel channel expansion method was devised to approximate the electronic wave functions. In spherical coordinates (the proton sits at the origin, see Fig. 1), total Hamiltonian and a generalized angular momentum operator are given by,

$$H = -\frac{1}{2} \frac{\partial^2}{\partial r^2} - \frac{1}{r} + \frac{\Lambda(r, \theta)}{2r^2}, \quad (1)$$

$$\Lambda = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + 2r^2 V(r, \theta).$$

The channel functions are defined as eigenstates of the generalized angular momentum operator at a give  $r$ . The channel functions are approximated by the Legendre polynomials for small  $r$ , and their distribution shrink in a restricted region of small  $\theta$  for larger  $r$  due to potential well of the metal surface,  $V$  in eq. (1). Two energy levels of  $n=2$  excited states above an aluminum surface were calculated taking only the first three channel functions into account. The energies at distance of 5 Bohr radius from the surface were obtained to be -0.075 a.u. and -0.044 a.u. (1 a.u.  $\approx 27.2$  eV), respectively, which are consistent with theoretical values reported by Kürpick et al.<sup>4)</sup> It is noted that the energy of  $n=2$  manifold for isolated H atoms is -0.125 a.u.

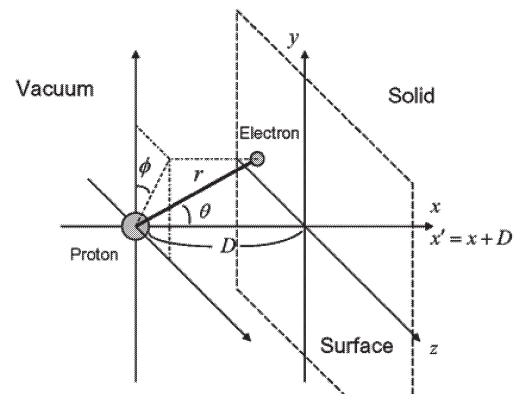


Fig.1: Spherical coordinates of electron. Proton sits at the origin.

### References

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