§20. Excited State Abundance in High-energy Neutral Hydrogen Atoms Reflected at Metal Surfaces

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Numerical methods were developed to study single electron capture by translating hydrogen atoms above metal surfaces. The present method gives predictions for hitherto unknown population distribution of excited species in hydrogen atoms reflected at the metal surfaces.

Previously, excited state population was observed by detecting photon emission from neutrals of an ion beam backscattered at metal surfaces for incident energies of a few keV or higher[1]. Some theoretical calculations have been conducted to explain the excited state population in terms of single electron transfer between excited atomic levels and conduction bands of metal surfaces. Burgdörfer et al. calculated n=2 population of atomic hydrogen specularly reflected with grazing angles at gold surfaces[2]. They adopted the kinematic resonance model for the electron transfer associated with nuclear translation parallel to the surface, while adiabatic approximation was used for electronic state evolution associated with the translation along the surface normal. Kato et al.[3] pointed out contribution of non-adiabatic promotion of the translating electron due to the nuclear motion along the surface normal in a simplified one-dimension system; geometry of the electronic system was restricted to the surface normal only.

In the present work, the previous works were extended to calculate distributions of the excited state population taking account of kinetic energy and angular distributions of backscattered hydrogen atoms. The present electron transfer model gives predictions for the excited state populations of hydrogen atoms translating above metal surfaces with a given velocity and emission angle to the surface normal. With the aid of Monte-Carlo simulation, the excited state distribution in reflected neutrals of a certain energy distribution and the given emission angle are obtained.

The excited state abundance was calculated for Mo surface. Kinetic energy distribution of the reflected atoms was taken into account with the aid of the Monte-Carlo simulation code (ACAT)[4]. Energy distribution associated with the $3d_2$ excited state (see Fig. 1) in reflected neutrals consistently explains peak energy variation with incident energies of Doppler-shifted D_α lines measured by Tanabe et al.[1] Occupation probability of the magnetic sub-levels is obtained to be highly polarized (see Fig. 2). It suggests strong anisotropy in angular distribution of photon emission from the excited states created via the surface electron capture.

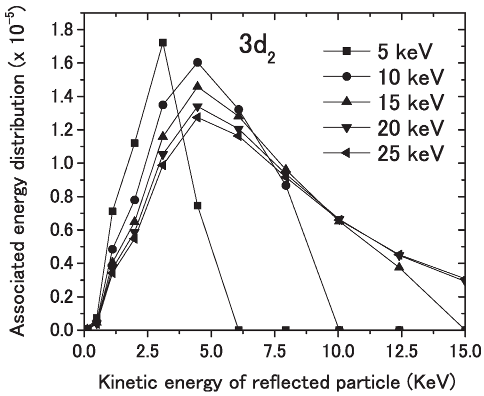

Fig. 1: Associated energy distribution of $3d_2$ state in neutral D atoms reflected at Mo surface with an emission angle of 60 degree to the surface normal. The distributions are shown for five incident energies in 5-25 keV and an incident angle of the 60 degree.

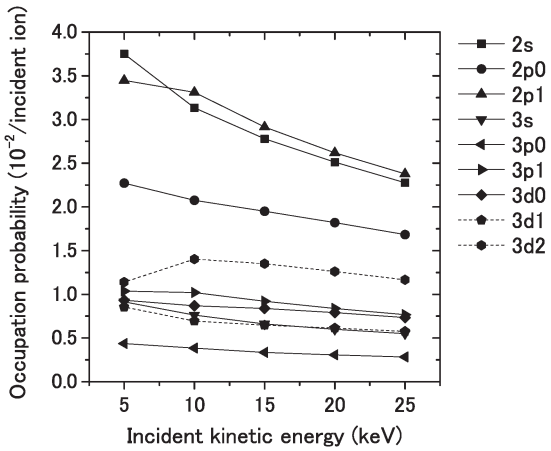

Fig. 2: Occupation probabilities of excited states in neutral D atoms reflected Mo surface with an emission angle of 60 degree to the surface normal.

1) Tanabe, T., Ohya, K., Otsuki, N.:J. Nucl. Mater. 220-222 (1995) 841.
2) Burgdörfer, J., Kupfer, E., Gabriel, H.: Phys. Rev. A 35 (1987) 4963.
3) Kato, D. et al.: J. Plasma Fusion Research 7 (2006) 183.
4) Yamamura, Y, Mizuno, Y.: IPPJ-AM-40, Inst. Plasma Phys., Nagoya Univ. (1985).