§19. Surface Adsorbed-impurity-plasma Interactions

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Charge transfer by ions, atoms and molecules from a solid surface plays a crucial role in a number of important physical processes, and inclusive are the sticking, desorption, and dissociation. In magnetic nuclear fusion devices, atomic and molecular states created via the charge transfer from surfaces of plasma facing components are important to understand behaviors of edge plasmas.

The charge transfer study also serves as a base for ion-beam electron-capture spectroscopy which is used as a powerful tool to investigate various properties of surfaces such as thermodynamic and critical behavior of surfaces, or magnetic and electronic characteristics not only from metals but also organic compounds. Recently, charge transfer shows a strong come-back as an urgent problem owing partly to the requirement of more high-resolution techniques from areas like plasma processing. It has been also a center of subject in astrochemistry where various molecules are known to form on the grain/surface of cluster in interstellar space.

There have been various theoretical attempts to study charge transfer from a surface. Despite these intensive efforts, there is still considerable lack of understanding of charge transfer processes. To contribute toward better understanding, we feel that it is necessary to investigate the subject with a unified effort from atomic and molecular physics and surface physics.

In this work, we investigated charge transfer from H or Na atom adsorbed on Al(100) surface by H^+ ion impact from 10 eV to 10 keV. H, Na and Al atoms have the Pauling electron-affinity value of 2.1, 0.9 and 1.5, respectively, and hence, for the [H-Al(100)] system, the electron charge distribution is pulled toward the adsorbed H atom from the surface, while for the [Na-Al(100)] system, it is reversed. Upon impinging H^+ ion on H or Na adsorbed surface, the incoming H^+ ion sees completely different environment near the surface, and therefore, it is extremely interesting to carry out a detailed comparative study of charge transfer dynamics between these two systems to answer some questions like why and how charge transfer would occur or not occur and what is the spin state after charge transfer. In the present calculation, Al atoms which constitute the surface are explicitly considered up to 72 atoms, in addition to adsorbed H or Na atoms, in the calculation of electronic states of the whole system and a semi-classical treatment for scattering dynamics is employed. Inclusion of a large number of atoms for mimicking the surface property properly is the first trial of this kind, as far as we know, and should be expected to provide more realistic information about charge transfer.

Probabilities for elastic scattering and charge transfer between the H^+ ion and the H- or Na-atom adsorbed Al(100) surface were calculated for incident kinetic energies between 10 eV and 10 keV. Charge transfer was found to take place significantly between the H^+ ion and the H atom, while it was suppressed in the case of the Na atom. We also studied the orientation and alignment of the cloud of the electron captured in 2p states by the H^+ ion.