# §18. Charged and Neutral Particle Behavior at and near Plasma Facing Material Surfaces

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In this working group, we investigate electronic excitation, ionization, electron capture, and electron emission at plasma facing material surfaces exposed to plasmas. It aims to understand energy and particle transport under abnormal circumstances such as arcing, hotspot etc. Theoretical methods and simulation codes which were developed in this project would be available for nuclear fusion researches at the NIFS.

One of research topics is excited state abundance in neutrals reflected at refractory metals. The excitation probabilities are expected to be important for spectroscopic diagnostics of high-energy hydrogen component reflected at the plasma facing wall. To estimate the excitation probabilities, a semi-classical theoretical method (electronic transition was treated quantum mechanically, while proton motion was represented by classical trajectories) is being developed. The method enables to calculate single-electron capture by a proton outgoing from metal surfaces. The calculations are being performed for tungsten, molybdenum, beryllium, etc. Preliminary results were presented at the 14$^{th}$ International Toki Conference joined with the 4$^{th}$ International Conference on Atomic and Molecular Data and Their Applications (Toki, Oct. 5-8, 2004)[1].

Monte Carlo program code of electron backscattering and secondary electron emission from solids has been published in NIFS-DATA series[2]. The program code was developed by the collaborator (Ohya), and is available for researchers on their request. The code is applicable to mono-atomic metals, semi-conductors and insulators for electron impact energies of 0.1 – 10 keV. It provides information on energy and angular distributions of backscattered electrons and secondary electrons, as well as total yield.

A quantum molecular dynamics code (VASP) has been introduced in this working group. The code is applicable to calculating accurate impurity transport coefficients in fusion reactor materials.

Two group meetings were held in January and March 2005 to discuss about each research topic. One of the meetings was held as a joint meeting with “theoretical and simulation study on boundary layer plasma” working group. Studies on secondary and backscattered electron emission from solid targets by charged particle impact were reviewed, and an effect of the electron emission on the ion sheath profile was examined at the meeting. In the other meeting, Prof. M. Tanaka (NIFS) was invited to present his quantum molecular dynamics study on chemical sputtering of graphite by hydrogen. Measurements of the chemical sputtering rate at the JT-60 were presented by the collaborator (Nakano). Current understandings on mechanisms of the chemical sputtering were reviewed at the meeting. It was suggested that transport coefficients of methane molecules in the graphite should be studied by using the quantum molecular dynamics.

References

1) Kato, D. et al.: submitted to Journal of Plasma and Fusion Research.
2) Ohya, K. et al.: NIFS-DATA 84 (2004).