§41. Theoretical Calculations of W Atomic Collision Processes Relevant Magnetic Nuclear Fusion Plasmas

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Tungsten is a prime candidate for plasma-facing component (PFC) materials of ITER and DEMO reactors. It is assumed that tungsten would prevent the PFC from serious radiation damage and tritium retention, since it has lower sputtering and hydrogen retention rates. Nevertheless, it is an issue of study if tungsten PFC still persists the feasibility under edge localized mode (ELM) and impurity gas feeding for radiation cooling of edge plasmas.

Recently, impurity holes have been observed in LHD operations; heavy impurity ions (e.g. C, Ne) are preferentially distributed in peripheral region. EUV spectra measured after tungsten injection using TESPEL at LHD also suggest small concentration of tungsten ions in core plasmas. To understand more detailed correlation between the measured EUV spectra and ion distributions (transport), it is necessary to acquire atomic collision data of tungsten ions in the plasmas. This collaboration studies were conducted to calculate new atomic data for ionization of tungsten atoms and ions by collisions with plasma particles including neutrals, and charge exchange of tungsten ions and atomic hydrogen.

Fig. 1 shows calculated total ionization cross sections of W^+ ion, which at present is one of the most interesting subjects for plasma impurity, by electrons, protons, neutral H and He atoms [1]. It is seen that at low energies, ionization by H and He prevails and the corresponding cross sections are extremely large. Influence of electron and proton components is important at rather high energies. At low energies, the main contribution to ionization is due to close collisions and the cross-section value is defined by overlapping volume of electron densities of two colliding particles. At high velocities, ionization cross section depends mainly on the Coulomb field created by target nucleus and electrons.

Tungsten ions have complicated electronic level structures due to many electrons in valence shells. This complexity makes *ab initio* calculations by standard atomic collision theories challenging. Quantum chemical approaches make it feasible to deal with such complex systems in solid footing manner. We have undertaken the quantum chemical calculations of potential energy diagrams of WH^+ molecules in order to calculate charge exchange between W^+ and H. Fig. 2 shows a preliminary result of the energy diagram as a function of inter nuclear distance of WH^+. In separated atom limit, all potential energy curves in the figure converge to energy levels of ^6D manifold of the ground state W^+ and H(1s). Calculations of higher energy levels of charge exchange products, i.e. W and H^+, are under progress. From these energy diagrams, primary insights of charge exchange probabilities can be obtained by analyzing their level crossings.

This work is supported by the NIFS/NINS project of Formation of International Network for Scientific Collaborations.

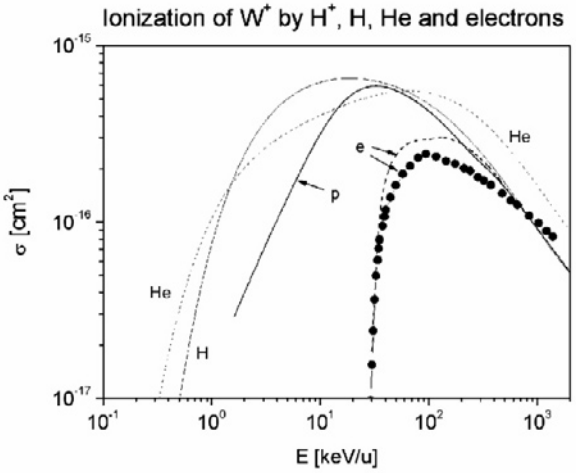

Fig. 1 Calculated total (a sum of single-, double-, triple etc. ionization cross sections) ionization cross sections of W^+ ions by electrons (e), protons (p), H and He atoms as a function of W^+ energy. Experiment: solid circles [2]. Theory: e – electron-impact ionization cross section, ATOM code; p – proton impact, LOSS code, H and He – ionization by H and He atoms, respectively, DEPOSIT and LOSS codes. Electron-impact ionization cross sections are shown as a function of equivalent electron energy for comparison.

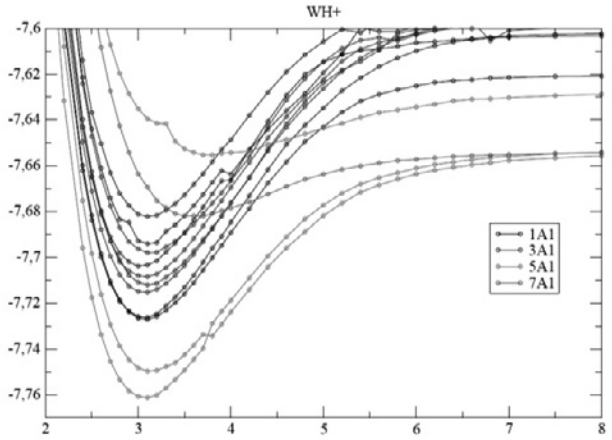

Fig.2 Energy diaglam of WH^+ as a function of inter-nuclear distance (in au). All potential energy curves in the figure converge to energy levels of ^6D manifold of the ground state W^+ and H(1s). Calculations were performed by using multi-reference configuration interaction method [3].

1) Shevelko, V.P., Kato, D., Tawara, H. and Tolstikhina, I.Yu., Plasma and Fusion Research 5 (2010) S2012.

2) Tawara, H. and Kato, M., NIFS-DATA-51 (NIFS, Japan, 1999).

3) Buenker, R.J. and Peyerimhoff, S.D., Theor. Chim. Acta. *39* (1975) 217.