§7. Atomic and Molecular Database of High Z Elements and Molecules for LHD Peripheral Plasma

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On the course of the continuous update of atomic and molecular databases at NIFS, a comprehensive data mining and compilation of atomic and molecular cross sections has been performed by the present working group. The database AMDIS for electron collisions and CHART for heavy particle collisions, respectively, were constructed over decades ago, and have been continuously updated from time to time. The databases AMOL and CMOL, which are extended for molecular targets have also been provided and maintained by NIFS. Updates and extension of these NIFS atomic and molecular database, especially for the data for atomic process with high Z elements, which are relevant for the LHD peripheral plasma, have been carried out in the present collaboration. In addition, extension of the NIFS database to include radiation induced atomic and molecular processes has been discussed.

i) Atomic data of high Z elements

Excitation-, ionization- and total-cross sections for electron collision with atoms and ions of high-Z elements, such as Fe, Ni, Mo, and W were surveyed from the literature. Survey of the cross sections for rare gas atoms, such as Ar, Kr, Xe were also carried out. Data for the electron – ion recombination processes were also surveyed. To prepare for the future modification of the database to accommodate rate coefficients, the relevant data on the rate coefficient have also been collected. New data from over hundred reference articles were added to the database AMDIS in the present project.

For the heavy particle impact cross section data for CHART, we have reviewed ions of H, He, Ne, Ar, Kr, and Xe impact on high-Z elements such as, Fe, Ni, Mo and W, in various charge states. Updates of the atomic and molecular database AMDIS and CHART for high-Z elements will be appear in NIFS-DATA[1].

It is found that most of the absolute cross section data for high-Z elements, a part from rare gas atoms, are obtained theoretically. Experimental cross sections are strongly demanded for reliability for the data for high-Z elements, which will be highly required for the plasma modeling in fusion science.

Recent literature research for cross section data also shows that number of experimental reports providing electronic state selective data, which will help to make a more realistic model for plasma diagnostics, are increasing for rare gas targets. However, the data are often relative quantities and most of these data were not included in AMDIS or CHART.

ii) Survey for the extension of the NIFS database to radiation induced atomic and molecular processes

Recently, atomic and molecular processes induced by the strong radiation from the LHD plasma are attracting more attention. Survey for the existence database of radiation induced atomic and molecular processes were performed. In addition, capability of the current NIFS database to include the atomic and molecular processes induced by radiation was discussed. As a part of this project, cross section data for photon induced processes, i.e. photoabsorption cross sections, photoionization cross sections, and photodissociaiton cross sections for some high Z elements and small molecules were surveyed.

iii) Updates of the database for electron impact cross section for hydrogen molecule

Construction of comprehensive set of electron impact cross section data for hydrogen molecule was attempted in the present project. Various experimental and theoretical data for electron impact cross sections for molecular hydrogen have been reported up to know. A complete survey for the existing literature and extraction of the cross section data sets were carried out in the present project. In addition, extensive compilation and evaluation of electron impact cross sections for molecular hydrogen have been reported, recently.[2] Including the evaluated data, comprehensive set of electron hydrogen molecule will be stored in AMOL.

iv) Updates of the database for molecular target electron impact cross section for hydrogen molecule

Continuous compilation of the database for electron impact and heavy particle impact cross section data on hydrocarbons are also the urgent issue. Recently, electron impact cross section data for small hydrocarbons were stored into the database.[3] Cross section data for heavy particle impact on small hydrocarbons were also compiled and stored.[2] Here we also initiated a joint experimental and theoretical investigation to produce and evaluate the cross section data for molecular targets.

1) Kitajima M. et al., NIFS-DATA, *in preparation*.
2) Yoon J.-S. et al. : J. Phys. Chem. Ref. Data 37 (2008) 913
3) Kimura M. et al. : NIFS-DATA-98 (2006)