§44. Atomic and Molecular Database of Hydrogen-isotopes and Hydro-Carbons

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Atomic and Molecular processes play an important role in fusion plasmas. The cross section database for collisions processes of elements consists the plasma facing materials are needed to model the transport of eroded atoms and molecules. Data compilation and evaluation of atomic and molecular cross section data for fusion research at NIFS have been continuously proceeding. 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. There also are databases for electron collisions and heavy particle collisions with molecules, so called AMOL and CMOL respectively. On the course of the continuous update of the atomic and molecular databases of NIFS, a working group has been organized for comprehensive data compilation of atomic and molecular cross sections. Recently, 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 by the working group.[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.

During the collaboration for the collection and compilation of atomic and molecular data for high Z elements, it was found that atomic and molecular data for electron impact and heavy particle impact cross section data on hydrogen isotopes and hydrocarbons are the urgent issue. Electron impact cross section data for small hydrocarbons, together with heavy particle impact cross sections on small hydrocarbons have been continuously surveyed our collaboration and stored into the database, up to year 2000.[2] However, new experimental as well as theoretical data for various processes by electron impact and heavy particle impact on hydrocarbons have been reported from since we have carried out data survey.

Compilation of the cross sections for the electron impact and heavy particle impact on hydrocarbons was attempted. Molecular targets such as fluorinated hydrocarbons are now coming to one of the most important issue in the plasma processing. The number of the cross section data on the plasma processing demanded targets including the fluorinated hydrocarbons is also increasing. In the present collaboration, however, we have primarily been concern with the atomic and molecular data on hydrocarbons.

In the present collaboration, a comprehensive data mining and compilation of atomic and molecular cross sections for the atomic and molecular processes including hydrogen isotopes and small hydrocarbons have also been attempted. 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.[3] Including the evaluated data, comprehensive set of electron hydrogen molecule will be stored in AMOL.

Here we also point out that during the last collaboration for the collection and compilation of atomic and molecular data for high Z elements, we found that the number of accurate cross section data are still very small, especially for the targets such as W[1]. This may be due to the experimental and theoretical difficulties in treating the high-Z targets for measuring and calculating its collision cross sections. However, there is an another fact that the number of the groups studying the atomic and molecular cross sections, especially in the absolute values, is decreasing. Since, the number of the experimental and theoretical cross section data is still insufficient for a large number of targets, it is important to encourage overcoming those difficulties in obtaining atomic and molecular cross sections.

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