

## §17. 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 these NIFS databases, a working group has been organized for comprehensive data compilation of atomic and molecular cross sections. 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. In this working group, we have constructed and started the plan for extending the database to include atomic process of high Z elements, which are relevant for the LHD peripheral plasma. Comprehensive survey for the cross section data of molecular hydrogen were also the planed.

### i) Atomic data of high Z elements

Compilation of the cross sections for the electron-impact excitation and ionization of atoms of high-Z elements for AMDIS was attempted. In the present project, we have paid attention to metal targets like Fe, Ni, Mo, and W. We also made survey for the rare gas atoms such as Ar, Kr, Xe. Wide range of the target charge states were considered. To prepare for the future modification of the database to accommodate rate coefficients, the relevant data on the rate coefficient have also been collected. Extensive and systematic calculations based on the R-matrix method were performed recently, and the cross section data from these studies were useful for reassess the accuracy of previous and new data.

For the heavy particle impact cross section data for CHART, we have reviewed  $H^+$  impact on high-Z elements such as, Fe, Ni, Mo and W, in various charge states.

### ii) Molecular targets

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. The data will be examined and stored in AMOL.

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.<sup>1)</sup> Cross section data for heavy particle impact on small hydrocarbons were also compiled and stored.<sup>1)</sup> In the present project, data sets from the extensive work on measurements of low energy cross section for ion impact cross sections in various molecules, carried out by one of the member,<sup>2)</sup> were compiled and stored into the database.

Here we also initiated a joint experimental and theoretical investigation to produce and evaluate the cross section data for molecular targets.

### iii) 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. We examined the capability of the current NIFS database to include the atomic and molecular processes induced by radiation. As a part of this project, cross section data for photon induced processes, i.e. photoabsorption cross sections, photoionization cross sections, and photodissociation cross sections for some high Z elements and small molecules were surveyed. Extensions of the NIFS database for radiation induced processes are in progress.

## References

- 1). M. Kimura et al., NIFS-DATA-98 (2006)
- 2). K. Okuno, NIFS-DATA-100 (2007)