

§21. 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. Updates and extension of the NIFS atomic and molecular database, including atomic process of high Z elements, which are relevant for the LHD peripheral plasma, have been carried out in the present collaboration.

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. More than a hundred data were newly added to the database AMDIS in the present project. It was also found that cross section data for electron-impact of Mo and W are still limited instead of its needs from the plasma modeling in fusion science.

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 of high-Z elements will be appear in NIFS-DATA.

ii) Updates of the database for 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 in the present project. In addition, extensive compilation and evaluation of electron impact cross sections for molecular hydrogen have been reported, recently.¹⁾ Including the evaluated data, comprehensive set of electron hydrogen molecule will be 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.²⁾ 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.

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. Examination of the capability of the current NIFS database to include the atomic and molecular processes induced by radiation was carried out. 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.

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