§ 1. Atomic Data Compilation and Update of the NIFS Databases

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Systematic efforts for revision and update of NIFS databases have been carried out for electron and ion impacts on various atomic and some molecular targets by a few experts on these fields. The original databases called AMIDIS for electron collisions and CHART for heavy-particle collisions, respectively, have been completed over decades ago, and from time to time, some efforts have been taken to update the databases. Since the last revision made sometime ago, probably more reliable data for various atomic and molecular systems at different collision energy range are now available. Therefore, new and systematic effort to update these databases is considered to be indispensable. For recent years, theoretically very extensive and accurate calculations based on the close coupling (CC) method with elaborate basis sets such as atomic orbitals (AOs) or molecular orbitals (MOs) have been performed routinely for inelastic processes, while experimentally very elaborate beam experiments can be carried out, in combination with various types of lasers, so that one can determine different scattering parameters fairly accurately. Consequently, significant progress for both areas has been made particularly since 1990. Therefore, we have felt it essential to reevaluate these new data critically and establish recommended values for electron and heavy-particle ionic impacts for the NIFS databases at least within last ten years or so.

Electron impact: Compilation of the cross sections for the electron-impact excitation and ionization of atomic ions was attempted. On the basis of the survey of literature, mainly those published since 1990, the excitation and ionization cross sections have been compiled and input into the database AMDIS. This time, particularly, we have paid attention to metal targets like Fe, Ni and so on. 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.

Heavy-particle impact: For ion impact, we have reviewed Li^{q+}, (where q = 1-3) impact, C^{q+} (q = 1-6) impact on H and He atoms, and H^+ impact on heavier metal targets such as W, Fe, Ni, Co and Cu from keV to meV collision energies. Hence, charge transfer and ionization cross sections thus evaluated are regarded as benchmark results, replacing old ones in the CHART. Particularly for C^+ impact on H atom, very accurate MOCC calculations for a single charge transfer for a wide range of the collision energy from 10 meV/u to 50 keV/u have been reported by Stancil et al., and these cross sections are very useful for various applications from fusion science to astrochemistry.

Continuing effort to collect and assess cross section data for molecular targets both for electron and ion impacts is underway where very many studies have been reported. Furthermore, we have completed a report of the progress of our activity and published as a NIFS report in early 2003.