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

Kimura, M. (Yamaguchi U.), Igarashi, A. (Miyazaki U.), Motohashi, M. (Tokyo U. Ag. and Tech.), Kusakabe, T. (Kinki U.), Morishita, T. (U. Elec-Comm.), Moribayashi, K. (JAERI), Kitajima, M. (Sophia U.), Imai, M. (Kyoto U.), Pichl, L. (Aizu U.), Kato, D., Murakami, I., Kato, T.

Continuing and 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 specialists on atomic and molecular collision physics. The original databases called AMDIS 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 by collecting those recently published, critically evaluating these data and implementing into these 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 important. For recent years, theoretically very extensive and accurate calculations based on the R-matrix method, and 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 for electronic and ionic impacts, while experimentally very elaborate beam experiments are also 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, particular attention has been paid to heavy-metal targets from Fe to Zn. We have also undertaken the effort to collect molecular targets such as H_2 and O_2. Extensive and systematic calculations based on the R-matrix method were performed recently for ionic targets by one of our members, and the cross section data from these studies were included in AMDIS.

Ion impact: For ion impact, we have reviewed H^+, B^{q+} (where q = 1-5), and C^{q+} (q = 1-6) impacts on H, He and heavier metal targets such as W, Fe, Ni, Co and Cu from keV to MeV collision energies, although very little investigation has been carried out for heavier targets. We have initiated new effort to collect and evaluate cross section data for molecular targets ion impact. This year, we have primarily been concerned with smaller hydrocarbons such as CmHn where m<2 and n<6.

Based on these investigations, we have completed a report of the progress of our activity and published as a NIFS report in early 2004. Another report is now in editing stage and soon will be published as an article in Journal of Physical and Chemical Data.