§24. Development of Internet Vertical Atomic and Molecular Database for Studies of Light Sources and Plasma Processing

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We have witnessed recent fast, significant and remarkable advancement in past decades in areas such as high-tech. industries, medical research, environmental science, atmospheric science, fusion sciences as well as other basic sciences including astrophysics and radiation physics and chemistry, which are fully depend on extensive utilization of atomic and molecular (A&M) data for basic understanding of various phenomena, but also establishing guiding new key principles and basic technologies based on simulations with this accurate and complete A&M data basis.

We held meetings on May 13, June 6 2014, and Mar. 19, 2015. We held a joint seminar on Sep. 11 –12 to discuss about present status and future prospect of A&M data, mainly for multiple-charged ions in the magnetic fusion and laser produced plasmas. Furthermore, members of the project organized a symposium titled “Atomic and radiative processes of multiple charged ions and their applications”, at the plasma2014 conference on 21 Nov. 2014.

In these activities, we realize that a significant progress has been made recently in the study of atomic processes of multiple charged ions.

For example, in the Large Helical Device (LHD) in NIFS, visible and EUV spectrum of W ions has been observed and the emission lines are identified through comparison with calculation using HULLAC and other atomic codes as well as charge specific spectroscopy carried out using EBIT. Theoretically, a large-scale atomic model has been developed[1)], with which the synthetic spectrum of W plasma is calculated, which enables one to perform a detailed comparison between experimental and theoretical ion abundance, and their dependence on the electron temperature is investigated. The results are also compared with those from previous experiments carried out at JT-60[2)] and ASDEX-upgrade[3)]. It is shown that calculated mean charge agree well with experiment at high temperature (>1keV) where near Ni-like ions have a large abundance. On the other hand, at low temperatures, present model overestimates the ion charge. These comparisons suggest that accurate rates of ionization and recombination of W plasmas are necessary especially for dielectronic recombination. Moreover, in order to combine the model of atomic processes with those for plasma wall interaction, to be useful for analyzing the throughout effect of W impurities in the fusion plasmas, atomic data of low charged W is essential. As those data is not available with existing atomic codes, suggesting that more investigations are needed to develop new idea of estimating atomic structure and cross sections.

We investigate atomic data and atomic processes for laser pumped plasma (LPP) extreme ultra violet (EUV) light sources. The EUV sources have been studied intensively toward realization of the next generation microlithography. Sn plasma is used for the source at the wavelength of 13.5nm, in which atomic and radiative processes of multiple charged ions are investigated, to improve efficiency and output power. For shorter wavelength sources for the future lithography and other applications, atomic processes of heavier elements are of the interest. Present atomic model is useful for predicting emission wavelength as well as plasma condition to obtain sufficient ionization stage of target ion. The characteristic feature of 4d-4f transitions of 4d open shell ions have already been well investigated, however, emission from lower charged ions with 4f open shell needs more investigation. In addition, the optimization of the source requires radiation hydrodynamics simulation, in which calculation of energy and angular resolved radiation transport is still a challenge.

These examples suggests that matching data producers and data users of the A&M data will be useful for such applications from light sources to plasma processing. Methods to estimate energy levels and rate coefficients are also useful to have a complete collisional radiative model in the case when accurate A&M data are not available. We investigate methods for the communication between data producers and data users based on the present internet technologies. For example, SNS (social network services) may provide efficient communication, however, interfaces specific to scientific uses may be needed. Development of a database of researchers including wish list of A&M data may also be useful. Although, development of the database has difficulties, taking the fact that a large amount of A&M data as well as corresponding publications have already been accessible through the internet into account, possible implementation of a portal to search engines using metadata should be considered.

[1] A. Sasaki et al., J. Phys. B46, 175701 (2013).
[2] T. Nakano et al., J. Nucl. Mater. 415, S327 (2011).
[3] T. Pütterich, et al., Nucl. Fusion, 50, 025012 (2010).