§3. Study on Methods for Scientific and Industrial Application of Atomic and Molecular Data

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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 undertook this collaborative effort to establish the forum as a platform connecting between A&M data producers and data users to integrate independent and isolated effort of data production and storage so that more efficient and complete data production and transmission could be possible, through the establishment of a non- profit organization (NPO), named "The Forum for the Atomic and Molecular Data And Their Applications".

We held meetings on Apr. 3, May 13,　June 6, July 10, and Oct. 2, 2013. We held a joint seminar on Oct. 30 – Nov. 1, 2013, with the collaboration for meetings of NIFS titled, "Seminar of the Forum of Atomic and Molecular Data And Their Applications on VAMDC (Virtual Atomic and Molecular Data Center)". Furthermore, members of the project presented invited talks at the symposium organized by the division of CVD reactions in chemical reaction engineering of the society of chemical engineering in Japan, on the atomic and molecular data for the simulation of the plasma processing on Sep. 6.

In these activities, we investigated technologies for the development and application of the atomic and molecular databases. The atomic data in existing databases are mainly collected and evaluated by hands thus it has been difficult to supply enough data to users in application fields. Since 2009 in the VAMDC activity has been carried out for the development of a worldwide database. The VAMDC is a Consortium of Databases & Services Providers that has built a unified, secure, documented, flexible and interoperable e-science environment-based interface to its members atomic and molecular databases [1]. Not only VAMDC has a portal (fig.1), which provides web interface of the database,　but provides standard format of atomic data called XSAMS based on the XML technologies. Tools for manipulating atomic data in XSAMS format for both data producers and data users are also developed by the contribution of community members, which will enable users to evaluate the data as well as develop the collisional radiative model automatically for application purposes. For instance, users can develop their own computer program, which submit queries to the VAMDC to download XML format data and converts the data to the user's format. VMADC is based on the idea of VO (Virtual Observatory), which has a policy of open use of data and software in the scientific community, which enables a large number of contributors to join the project for the development of large database and improvement of quality of the data in the database.

In the study of W plasmas for fusion applications it is realized that a large-scale collisional radiative model should be developed, which should also be validated through systematic sensitivity studies [2-4]. The atomic model is developed using an algorithm, which is also used to calculate wavelength and radiative rates of emission lines concerning to a large number of atomic energy levels. Significant effort has also been carried out for the investigation of the mathematical and computational methods in ADAS project [5]. These show increasing demands of computational technologies for accurate and efficient processing of atomic data.

(fig.1) VAMDC portal [1].
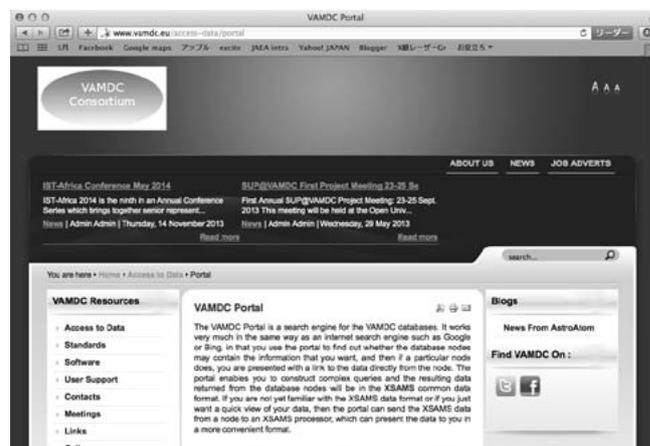
1) http://www.vamdc.eu/index.php
2) A. Sasaki, High Energy Density Phys. **9**, 325 (2013).
3) A. Sasaki and I. Murakami, J. Phys. B46, 175701 (2013).
4) A. Sasaki and I. Murakami, Plasma Fusion Res. 8, 2401021(2013)
5) http://www.adas.ac.uk