Determination of Atomic Data Pertinent to the Fusion Energy Science Program

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Final Report for the years 2011 – 2014

The objective of this program was to provide atomic data that needed for the DOE fusion energy science program. The main focus was on data for ITER, although needs of other tokamaks and fusion devices were not overlooked. During over 40 years of its existence, the program maintained extensive relations with the fusion energy community. Examples are our extensive collaborations with IAEA, non-LTE Workshops, and XML data exchange committees. This report covers our activities for the last contract period 2011-2014. Reports for previous years have been submitted as progress reports at regular intervals over the years. As our results for the recent period have been very extensive, this report only covers a sampling of our work during this time. The results are given separately for the primary areas that we covered.

1. **Identification of Spectral Lines of Impurity Ions.** Several important papers on Mo and W based on laboratory spectroscopy with electron beam ion traps (EBITs) and spark light sources and high resolution spectrometers were published. These are common wall materials in tokamaks. This research is based on high-precision spectroscopic measurements accompanied by large-scale collisional-radiative modeling of EBIT and other plasmas. To cite a few examples:

Extreme Ultraviolet Spectra from N-Shell Ions of Gd, Dy and W,
D. Kilbane, J. D. Gillaspy, Yu. Ralchenko, J. Reader, and G. O'Sullivan,
Phys. Scr. **T156**, 014012 (2013)
Magnetic-Dipole Transitions in Tungsten and Other Heavy Elements Observed with the NIST EBIT,
J. Reader, J. D. Gillaspy, D. Osin, and Yu. Ralchenko,
AIP Conf. Proc. **1438**, 86–90 (2012)
Spectroscopy of Diagnostically Important Magnetic-Dipole Lines in Highly Charged $3d^n$ Ions of Tungsten,
Yu. Ralchenko, I. N. Draganić, D. Osin, J. D. Gillaspy, and J. Reader,
Phys. Rev. A **83**, 032517 (2011)

2. **Spectroscopic Data Assessment and Compilations.** A major part of our program consisted of the critical compilation energy levels, wavelengths, and transition probabilities for the spectra of elements that are found in fusion plasmas. This included spectroscopic data for wall materials as well as gas that can be injected for diagnostic purposes as well as control of edge plasmas. Some examples:

Notes on Critical Assessment of Theoretical Calculations of Atomic Structure and Transition Probabilities,
H.-K. Chung, P. Jönsson, and A. Kramida,
Atoms **1**, 14–16 (2013)
Recent Progress in Spectroscopy of Tungsten,
A. Kramida,
Can. J. Phys. **89**, 551–570 (2011)

3. **Development of Online Atomic Databases.** During recent years we developed a number of online databases that provided an easily accessible source of atomic data to fusion researchers. We greatly expanded the content of our Atomic Spectra Database (ASD) and merged it with our bibliographic databases. We added material, with constant emphasis on fusion-related data. Material for negative ions was also added. We developed a number of web-based computational tools for support of magnetic and inertial fusion research, such as the plasma-kinetics code FLYCHK, and a new online collisional-radiative time-dependent code. Currently, the total number of energy levels and spectral lines in ASD is about 107,000 and 215,000, respectively. ASD is the only database in the world that contains recommended and evaluated data for atomic structure parameters. ASD can be access at the URL `http://www.nist.gov/pml/data/asd.cfm`.

4. **Collision and Spectroscopy Experiments with Highly Charged Ions on EBIT.** The NIST EBIT was extremely productive, with numerous papers on W and other fusion related elements (Hf, Ta, Au, Fe, Xe). We expanded the range of elements about tungsten to provide a more stringent test of theory and to achieve more accurate modeling. Some examples of papers that were published:

EUV Measurements of Kr XXI–Kr XXXIV and the Effect of a Magnetic-Dipole Line on Allowed Transitions,
Y. A. Podpaly, J. D. Gillaspy, J. Reader, and Yu. Ralchenko,
J. Phys. B **47**, 095702 (2014)

Magnetic-Dipole Lines in $3d^n$ Ions of High-Z Elements: Identification, Diagnostic Potential and Dielectronic Resonances,
Yu. Ralchenko, J. D. Gillaspy, J. Reader, D. Osin, J. J. Curry, and Y. A. Podpaly,
Phys. Scr. **T156**, 014082 (2013)

Anisotropic LMN Dielectronic Resonances from Ratios of Magnetic-Dipole Lines,
Yu. Ralchenko and J. D. Gillaspy,
Phys. Rev. A **88**, 012506 (2013)

Transition Energies of the D Lines in Na-like Ions,
J. D. Gillaspy, D. Osin, Yu. Ralchenko, J. Reader, and S. A. Blundell,
Phys. Rev. A **87**, 062503 (2013)

Extreme Ultraviolet Spectra of Highly Charged Xenon Observed with an Electron Beam Ion Trap,
D. Osin, J. Reader, J. D. Gillaspy, and Yu. Ralchenko,
J. Phys. B **45**, 245001 (2012)

EUV Spectral Lines of Highly-Charged Hf, Ta and Au Ions Observed with an Electron Beam Ion Trap,
I. N. Draganić, Yu. Ralchenko, J. Reader, J. D. Gillaspy, J. N. Tan, J. M. Pomeroy, S. M. Brewer, and D. Osin,
J. Phys. B **44**, 025001 (2011); Erratum: **44**, 179801 (2011)

5. **Electron Impact Collision Theory and Modeling of Plasma Spectra.** We developed advanced collisional-radiative models for diagnostics of emission spectra from fusion plasmas. This entailed (a) determination of spectroscopic data (energy levels and *f* values) for excited states of fusion-related atomic ions, (b) simulation of EBIT spectra measured in

our group, and (c) application of our time-dependent collisional-radiative model for charge-exchange-recombination-spectroscopy (CXRS) and motional Stark effect experiments. We developed an accurate time-dependent collisional-radiative model for CXRS diagnostics of tokamak impurities. Some examples:

Atomic Data for Beam-Stimulated Plasma Spectroscopy in Fusion Plasmas,
O. Marchuk, Yu. Ralchenko, D. R. Schultz, W. Biel, T. Schlummer, and TEXTOR team,
AIP Conf. Proc. **1545**, 153–163 (2013)
Benchmark of Collisional-Radiative Models for ITER Beams at the Alcator C-Mod Tokamak,
I. O. Bespamyatnov, W. L. Rowan, K. T. Liao, O. Marchuk, Yu. Ralchenko, and R. S. Granetz,
Nucl. Fusion **53**, 123010 (2013)
Comparison and Analysis of Collisional-Radiative Models at the NLTE-7 Workshop,
H.-K. Chung, C. Bowen, C. J. Fontes, S. B. Hansen, and Yu. Ralchenko,
High En. Dens. Phys. **9**, 645–652 (2013)
Non-Statistical Simulations for Neutral Beam Spectroscopy in Fusion Plasmas,
O. Marchuk, Yu. Ralchenko, D. R. Schultz, E. Delabie, A. M. Urnov, W. Biel, R. K. Janev, and T. Schlummer,
AIP Conf. Proc. **1438**, 169–174 (2012)
A Non-Statistical Atomic Model for Beam Emission and Motional Stark Effect Diagnostics in Fusion Plasmas,
Yu. Ralchenko, O. Marchuk, W. Biel, T. Schlummer, D. R. Schultz, and E. Stambulchik,
Rev. Sci. Instrum. **83**, p. 10D504 (2012)
Non-Statistical Population Distributions for Hydrogen Beams in Fusion Plasmas,
O. Marchuk, Yu. Ralchenko, and D. R. Schultz,
Plasma Phys. Controlled Fusion **54**, 095010 (2012)

In addition to peer-review journals, the results obtained during the contract period were disseminated in invited and contributed talks at a number of conferences, e.g.:

- International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA), Gaithersburg, MD, 2012
- CAARI-2012, Fort Worth, TX, 2012
- Non-LTE Code Comparison Workshops, Vienna, Austria (2011) and Santa Fe, NM (2013)
- International Workshop on Radiative Properties of Hot Dense Matter, Santa Barbara, CA, 2012
- ADAS Workshop, Auburn, AL, 2011
- International Conference on Atomic Processes in Plasmas, Belfast, UK (2011) and Mons, Belgium (2013)
- APS DAMOP meetings, 2011-2013
- International Conference on Physics of Highly-Charged Ions, Heidelberg, Germany, 2012
- International Toki Conference, Toki, Japan, 2012
- ITER-IAEA-ICTP Joint Workshop on Fusion Plasma Modeling using Atomic and Molecular Data, Trieste, Italy, 2012