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Data Evaluation for Heavy Particle Collision Processes

Summary Report of an IAEA Consultants Meeting

IAEA Headquarters, Vienna, Austria

17-18 March 2016

Prepared by

Hyun-Kyung Chung and Bastiaan J. Braams

April 2016

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Abstract

A Consultants' Meeting (CM) on Data evaluation for Heavy Particle Collision Processes was held in the IAEA headquarters in 17-18, March 2016 as a preparatory meeting for a coordinated research project (CRP) on the topic of Data for Atomic Processes of Neutral Beams in Fusion Plasma. Five experts participated in the meeting to give advices on the most important data of heavy particle collisions needed for fusion applications and discussed the current status of sources and quality of the heavy particle collisional data. The conclusions from the meeting will be used in the proposal of the CRP on Data for Atomic Processes of Neutral Beams in Fusion Plasma.

April 2016

TABLE OF CONTENTS

1. Introduction

A Consultants' Meeting (CM) on Data evaluation for Heavy Particle Collision Processes was held in the IAEA headquarters Vienna, from 17 to 18 March 2016. The objective of this meeting was to evaluate currently available atomic and molecular data for heavy particle collisions required by neutral beam diagnostics heavily used in fusion applications.

Neutral beam injection is a standard method to heat the plasma in fusion experiments and it is intended to be used for power control in ITER and perhaps in a reactor. Neutral beams also have important diagnostic uses, both via photoemission from the beam neutrals due to interaction with the plasma and via photoemission from plasma impurities after interaction with the beam. Modelling of the beam penetration into the plasma and of the spectroscopic signals relies on detailed data for atomic processes that involve the neutral beam particles. In spite of the importance of the data there are quite significant gaps, especially related to processes starting from an excited state of the neutral atom. On the other hand, for processes starting from the ground state of the neutral atom there are often several different families of calculated or measured data, obtained using different approximations or experimental methods, and it is important to assess their uncertainties and to recommend best data. A CRP on data for atomic processes of neutral beams in fusion plasma is proposed to provide evaluated and recommended data for the principal atomic processes relevant to heating and diagnostic neutral beams in fusion plasmas.

Five experts were invited to provide current status of heavy particle collision data and give an advice to the Unit about the scope of a CRP: N. Hawkes (Culham Center for Fusion Energy, UK), D. Schultz (University of North Texas, USA), T. Kirchner (York University, Canada), D. Reiter (Forschungszentrum Jülich GmbH, Germany) and X. Urbain (Université Catholique de Louvain, Belgium). D. Reiter and X. Urbain attended the final Research Coordination Meeting (RCM) on Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma, 14-16 March 2016 and extend one day to participate in this meeting.

Current status of data needs, available data and databases were reviewed by participants on the first day. On the second day, the scope of the CRP on data for atomic processes of neutral beams in fusion plasma and potential participants were discussed.

This report contains the proceedings of the meeting, conclusions and future work. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. Proceedings of the Meeting

B. Braams, the Head of Atomic and Molecular Data Unit in the Nuclear Data Section opened the meeting and reviewed the meeting objectives. The first day was mostly devoted for presentations and related discussions. N. Hawkes reviewed atomic physics data requirements for beam-plasma modelling in fusion experiments. D Reiter discussed the high energy asymptotics of cross sections and multi-parametric dependencies in effective data relevant for neutral beam injection. D. Schultz described the available charge transfer and excitation cross sections for CXRS and beam emission diagnostics and T. Kirchner presented theoretical descriptions of charge-transfer collisions involving few-electron systems. X. Urbain reviewed the total, partial and differential cross sections with light ion beams: past and present experimental techniques. Summaries of presentations are provided below.

The second day was devoted to define the scope of the CRP on data for atomic processes of neutral beams in fusion plasma and to write the preliminary proposal of the CRP.

Beam-plasma atomic data needs for fusion devices
N. Hawkes

Modelling of the attenuation of heating and diagnostic H/D/T beams in fusion plasmas is important for calculating the transmission of beam power through the plasma and the potential for damaging heat loads on machine structures. Uncertainties in attenuation of the ITER diagnostic beam by the time it reaches the centre of the plasma are acknowledged in the design of the charge-exchange diagnostic which will measure both beam emission (as a diagnostic of the local neutral beam density as well as impurity charge exchange. However, the calculated beam transmission affects the anticipated signal levels in the centre of the plasma and hence the signal-to-noise performance projected for the diagnostic. Good cross-section data for the impurity charge-exchange and beam emission processes are required for the quantitative analysis of these spectra. (Lineshape analysis—Doppler shift and broadening—is potentially affected by the fine structure of the impurity emission lines but these effects are insignificant at the temperatures of interest.)

Simulations of the D-alpha spectrum from tokamaks (developed to study the emission spectrum due to charge-exchange between fast deuterons and D heating beams—Fast Ion D-alpha—FIDA) need to accurately model the spectrum due to all processes. Among these is charge-exchange between D+ and D0 at the plasma edge for which state resolved cross-sections are needed.

The Motional Stark effect (beam emission) is applied on many Tokamaks with polarisation measurements used to measure the local magnetic field directions. Alternative measurements that use the intensity ratios of the sigma and pi lines depend on there being a given ratio of the populations of the upper states, any perturbation from statistical population would affect the interpretation.

Neutral lithium beams with energies of order 60keV are used in many fusion experiments to measure the edge electron density profile through the rate of attenuation of the beam. In fusion experiments with a lithium coated first wall the intrinsic lithium emission from the plasma can blind the beam diagnostic. In these cases the use of sodium neutral beams is being explored. Thermal energy helium gas jets are used in some experiments as a simpler alternative to the lithium/sodium. The rate processes for beam attenuation, excitation and charge-exchange for these injected neutrals are needed for the quantitative interpretation of the emission spectra.

Reionisation of heating beam neutrals can occur due to collisions with neutral gas in the ducts of the beam systems. At high neutral pressures this can lead to sufficient density of ionised particles as to pose a risk to machine components when the particles enter the plasma confining fields. Atomic data would be needed to model this process.

Atomic Data for CXRS and BES/Stark Diagnostics
D. R. Schultz

Several projects carried out recently were described illustrating the large scale calculation of data relevant to neutral beam heating/diagnostics in fusion experiments. For example, work to produce state-selective charge transfer data for CXRS involving Ar were described. First treated comprehensively in the 1990's [1] data were computed for $Ar^{15\text{-}18+}$ + H(1s), tabulating the n- and nl-resolved charge transfer cross sections for several energies relevant to neutral beam diagnostics at the time. The data were disseminated via the website of the ORNL Controlled Fusion Atomic data Center [2]. With an eye to ITER relevant neutral beam energies, this database was extended about ten years later to include higher impact energies, and also excited state H targets (H(2s), H(2p)) [3,4].

The method used to compute these data (again, recalculated for the relevant beam energies) was stringently tested by spectroscopic experiments at TEXTOR [5] confirming the results, and thus showing their utility for interpretation of CXRS measurements at present devices and for ITER. Similar work was also shown regarding the feasibility of CXRS for ITER using W^{64+} [6]. In this work, it was found that a number of strong lines arising from charge transfer with a neutral hydrogen beam in the VUV visible spectral range should be available for diagnosis of the likely most abundant tungsten ion in ITER core plasma. The results were obtained using newly calculated state-selective charge transfer cross sections and a detailed collisional-radiative model including thousands of levels populated by either electron-impact or charge transfer with the neutral beam.

Finally, relevant to beam emission spectroscopy and motional Stark effect spectroscopy, data and collisional-radiative modeling were reviewed that recently showed that the typical statistical assumptions about state distributions in plasma are not valid [7], point the way toward more complete ability to utilize neutral hydrogen beam excitation in diagnostics. Data for that work [8], consisting of full density matrix elements for H^+ exciting H(1s) to levels within n=2,3, and 4, from a few hundred eV to 2 MeV collision energies, provided during work of a previous IAEA CRP.

[1] Whyte, Isler, Wade, Schultz, Krstic, Hung, and West, Phys. Plasmas 5, 3694 (1998)
[2] www-cfadc.phy.ornl.gov/eprints/argon.html
[3] Schultz, Lee, and Loch J. Phys. B 43, 144001 (2010)
[4] www-cfadc.phy.ornl.gov/eprints/argon2.html
[5] Schlummer, Marchuk, Schultz, Bertschinger, Biel, Reiter, and the TEXTOR team, J. Phys. B 48, 144033 2015.

Charge-transfer collisions involving few-electron systems
T. Kirchner

Ion-atom collision systems that involve more than one electron constitute nonseparable few-body problems, whose full solution is difficult to say the least. At impact energies well below 1 keV/amu an expansion of the stationary scattering wave function in terms of a limited number of products of nuclear and molecular state wave functions (amended to satisfy scattering boundary conditions) is feasible and usually sufficient to obtain accurate charge-transfer cross sections provided the electronic wave functions include configuration interaction (e.g. [1]).

At energies above 1 keV/amu this approach becomes inefficient and close-coupling methods within the semi classical approximation are better suited to treat the problem. For bare-ion collisions from helium target atoms explicit solutions of the two-electron time-dependent
Schrödinger equation can be achieved, but are computationally costly and cannot be extended to problems which involve more than two electrons.

Approximate alternatives are thus necessary to deal with more general situations. The independent electron model (IEM) represents a convenient and often quite accurate framework to carry out charge-transfer calculations for many-electron collision systems. We have used the IEM, e.g., to calculate (n,l)-specific cross sections for single capture in Ne^{10+} impact collisions with He, Ne, and Ar atoms. One motivation for this work has been the availability of experimental data for Lyman α and Lyman β+ emissions after shell-specific single capture. When coupled with radiative cascade calculations our IEM results show good overall agreement with the measurements [2].

Time-dependent density functional theory provides a firm footing of the IEM and gives some hints of how to improve the calculations. In this context, we have investigated the use of correlation integrals in the final-state analysis of one- and two-electron processes in proton and He^{2+}- He collisions [3]. Particularly for the case of double capture, for which the IEM has the tendency to overestimate the cross section, this has improved the agreement with experimental data.

[1] L. F. Errea et al., J. Phys. Conf. Ser. **576**, 012002 (2015)
[2] A. C. K. Leung and T. Kirchner, Phys. Rev. A **92**, 032712 (2015)
[3] M. Baxter and T. Kirchner, Phys. Rev. A **93**, 012502 (2016)

High energy asymptotics of cross sections and multiparametric dependencies in effective data relevant for neutral beam injection
D. Reiter

The possible scope of a new CRP on atomic data relevant for neutral beam injection (NBI) should be to constrain and focus on the data issues to all processes relevant when the beam particles have left the sources, which include beam interacting Maxwellian electrons as penetrating plasma edge. The special attention is needed for cross-sections at high energy regions and asymptotic behaviors. Currently available data sets of some relevant processes such as heavy particle collisions involving He and metastable He are lacking the correct asymptotic behaviors at low and high energies.

It is recommended that underlying raw data of NBI important for ITER project should be publically exposed in a way as unprocessed as possible. Tools for producing multi-parametric beam stopping rates should be considered to be embedded into codes instead of reduced tables. The approximate method of scaling state resolved cross-sections for heavy particle data from electron impact data should be examined for its validity. It is important to benchmark collisional-radiative codes for NBI processes and the series of non-LTE kinetics workshops offer a good example. Sensitivity studies of 1D (time or 1 spatial coordinate) should be analytically possible as demonstrated by HYDKIN sensitivity module. For charge exchange process between diagnostic neutral beam of 100 keV (~ 1.5 MW) and impurities (C, Be, W, He, N, Ne, Ar) in ITER, it is necessary to identify W lines that are near the CX lines of interest.

3. Conclusions and Recommendations

The main outcome of this CM was a recommendation to proceed with a CRP with the focussed goal to provide comprehensive evaluated and recommended data for atomic processes of heating and diagnostic neutral beams of hydrogen (including the deuterium isotope) in fusion plasma. In part this is a data development activity and in part it asks for evaluation of existing data or of data that can be easily generated. The CM also advised about some topics in the vicinity of the main goal.

- Data for excitation and emission from neutral beam; BES (Beam Emission Spectroscopy), MSE (Motional Stark Emission)
- Data for CXRS (Charge Exchange Recombination Spectroscopy)
- High energy processes in the beam box
- Helium beams or helium gas injection
- Modelling
- Code comparison exercise on beam transmission and beam emission

It was recommended that low energy processes relevant for generation of the positively or negatively charged precursor beam should be outside the scope of the new CRP, as there is not much synergy between study of these low energy processes and study of the processes in the main plasma. It was also recommended that high energy collision processes in the beam neutralizer should be admitted in the scope of the CRP, but without requiring complete coverage. (The reason to de-emphasize study of these processes is that the design and operation of the neutralizer is likely to be driven by technology considerations without a critical role for detailed atomic data.) Concerning neutral beams of other elements, the CM advised to include data for processes of neutral beams of helium and lithium in the scope of the CRP, because in many cases similar methods are used and the same people are doing relevant work. However, the CRP would not set a goal to provide comprehensive data for elements other than hydrogen.

It was recommended that the CRP should provide data in as unprocessed a form as is reasonable in order to allow detailed kinetic modelling and to allow the development of applicable collisional-radiative models. Thus, for any collision process the CRP should provide density matrix elements or cross sections rather than rate coefficients; the user of the data can do the integration to obtain the rate coefficients for the relevant plasma conditions. Likewise, when a model provides state-resolved data then these are the primary output for the CRP; the user can do the appropriate averaging over incoming states and the sum over outgoing states when that is desired.

The relevant primary energy for neutral beam injection ranges from about 100 keV to 1 MeV and the relevant plasma temperature ranges from about 100 eV in the edge plasma to a few keV in the core plasma for present experiments and up to 20 keV in expected ITER operation; higher plasma temperatures, up to 40 keV, are created already in present experiments under special conditions.

A heating or diagnostic neutral beam is surrounded by "halo" neutrals from charge exchange processes and these have a typical energy corresponding to the plasma ion temperature. Taking into account the halo neutrals the CRP should provide cross sections appropriate for neutral particle energies in the range of 1 keV to 1 MeV. For collisions with electrons, taking into account a high-energy tail on the Maxwellian, we ask for cross sections for electron energies in the range of 100 eV to 100 keV.

The objectives of the CRP include uncertainty assessment and evaluations of the propagation of uncertainties in atomic data to plasma simulations. In the specific research objectives (enumerated below) each set of data development objectives is preceded by a sensitivity assessment of typical uses of the atomic data to uncertainties in those data. It was recommended to organize some plasma code comparison activities as a part of the CRP, comparing different calculations of beam penetration, beam photoemission and beam-based impurity spectroscopy in order to expose the dependence of the simulations on relevant atomic data and to prioritize data development and evaluation activities.

List of Participants

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<u>Appendix 2</u>

IAEA Consultants' Meeting on

Data evaluation for Heavy Particle Collision Processes

17-18 March 2016, IAEA Headquarters, Vienna, Austria

Meeting Agenda

<u>Thursday 17 March 2016</u> **Meeting Room:M0E61**

09:30 – 09:45 Opening, Introduction of Participants, Adoption of Agenda

09:45 – 10:00 **Bas Braams** "Meeting Objectives"

10:00 – 10:30 **Nick Hawkes** "Atomic physics data requirements for beam-plasma modelling in fusion experiments"

10:30 – 10:50 *Coffee break*

10:50 – 11:20 **Detlev Reiter** "High energy asymptotics of cross sections and multiparametric dependencies in effective data relevant for neutral beam injection"

11:20 – 12:30 Discussion on Heavy Particle Collision Data Needs for fusion applications

12:30 – 14:00 *Lunch*

14:00 – 14:30 **David Schultz** "Charge transfer and excitation cross sections for CXRS and beam emission diagnostics"

14:30 – 15:00 **Tom Kirchner** "Charge-transfer collisions involving few-electron systems"

15:00 – 15:20 *Coffee break*

15:20 – 15:50 **Xavier Urbain** "Total, partial and differential cross sections with light ion beams: past and present experimental techniques"

15:50 – 17:00 Evaluation of Currently Available or Unavailable Heavy Particle Collision Data

19:00 *Social Dinner*

<u>Friday 18 March 2016</u>

09:00 – 10:30 Review of on Heavy Particle Collision Data Needs for fusion applications

10:30 – 10:50 *Coffee break*

10:50 – 12:20 Review of Heavy Particle Collision Data Evaluation

12:20 – 14:00 *Lunch*

14:00 – 15:20 Definition of Coordinated Research Projects (CRP) on "Data for Charge Transfer Processes Related to Neutral Beams in Fusion Plasma"

15:20 – 15:40 *Coffee break*

15:40 – 17:00 Write-Up of White Paper on the CRP

17:00 – *Adjournment of Meeting*

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