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ATOMIC DATA FOR FUSION PLASMA MODELLING

Summary Report of an Advisory Group Meeting
on Atomic Data for Fusion Plasma Modelling
organized by the International Atomic Energy Agency
and held in Vienna, Austria,
18-20 September 1985

Prepared by J.G. Hughes
Nuclear Data Section
International Atomic Energy Agency

January 1986

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

This is a summary report of an Advisory Group meeting on Atomic Data for Fusion Plasma Modelling convened by the Nuclear Data Section of the International Atomic Energy Agency at IAEA Headquarters, Vienna, Austria, 18-20 September 1985. The meeting was held on the recommendation of the International Fusion Research Council Subcommittee on Atomic and Molecular Data for Fusion, to review the available atomic collision data relevant to fusion plasma modelling, with emphasis on processes involving iron and its ions. Fourteen experts from five Member States attended the meeting, representing the most active research groups in both the atomic collision physics and plasma modelling communities. The participants reviewed the status of data in the relevant areas of atomic physics and made specific recommendations regarding the use of these data in plasma modelling calculations.

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A. Meeting Summary

An Advisory Group meeting on Atomic Data for Fusion Plasma Modelling was convened by the Nuclear Data Section of the International Atomic Energy Agency at IAEA Headquarters, Vienna, Austria on 18-20 September 1985, on the recommendation of the International Fusion Research Council Subcommittee on Atomic and Molecular Data for Fusion. The purpose of the meeting was to review the available atomic collision data relevant to fusion plasma modelling, with emphasis on processes involving iron and its ions. Fourteen experts from five Member States attended the meeting, representing the most active research groups in both the atomic collision physics and plasma modelling communities. The participants reviewed the status of data in the relevant areas of atomic physics and made specific recommendations regarding the use of these data in plasma modelling calculations.

J.G. Hughes was Scientific Secretary of the meeting, while the individual sessions were chaired by D.H. Crandall, H.W. Drawin, M.F.A. Harrison and A. Miyahara. The meeting was opened by Professor V.I. Ferronsky, Director of the Division of Research and Laboratories, IAEA.

B. Meeting Proceedings

The interests of fusion plasma modellers in Fe collision data were reviewed by participants from some of the major fusion research laboratories, namely H.W. Drawin (CEA), R.A. Hulse (PPPL), J. Wiley (Texas), G. Fussmann (ASDEX), and T. Kato and T. Kawamura (Nagoya). The introductory presentation was given by Dr Drawin in which he gave a comprehensive review of the atomic data requirements for fusion plasma modelling.

Dr Kawamura discussed the effects of accuracy of atomic data in impurity transport modelling based on a one-dimensional tokamak model. As an example the difference between the results using different dielectronic recombination rate coefficient formulas was analysed, and it was concluded that in order to draw out reliable evidence of anomalous impurity transport considerably accurate atomic data is needed.

Dr Wiley reported new measurements of Fe injection and impurity transport carried out at TEXT, partly in preparation for this meeting. The TEXT transport results followed previous studies but new absolute intensity measurements with the calibrated grazing incidence system (GRITS) do not agree with modelling calculations. One possible reason for this is that the excitation rates used in the modelling are inaccurate.

Dr Kato discussed the effects of multistep ionization and K-shell ionization on the ion abundances and the rate of radiation loss necessary for plasma modelling of tokamaks. These processes have received relatively little attention

from plasma modellers but it was shown that under certain circumstances they become as important as direct ionization and excitation-autoionization.

Dr Hulse described the atomic data needs of the most critical areas of fusion plasma modelling, namely radiation power balance modelling and modelling of diagnostic signals. He also gave a very useful and enlightening description of the most appropriate format for the presentation and dissemination of compiled atomic data to the plasma physics community.

The important areas of atomic collision physics were expertly reviewed by the following participants : Prof. A.E. Kingston on electron impact excitation : Dr M.S. Pindzola on electron impact ionization ; Dr H.P. Summers on electron-ion recombination ; Dr R.A. Phaneuf on charge exchange. Prof. Kingston reported that high quality theory has been applied to calculate the excitation cross sections for a very large number of transitions in Fe ions. There is reasonable accord between different theories in most cases, even when resonances contribute significantly to the cross section. Considerable work is required however, to compile and parameterize these data.

For electron impact ionization Dr Pindzola reported new measurements by the ORNL experimental group for several ions of Fe, namely Fe(5+), Fe(6+), Fe(9+) and Fe(11+). Good measurements are also available for Fe(+) and Fe(2+). In some cases the crossed beams experiments demonstrate the significant influence on the total ionization cross section of excitation-autoionization processes and of the presence of metastable ions in the beam. However the effect of excitation-autoionization has been accurately predicted for some ions and can be roughly estimated for all the ions of Fe.

Dr Summers reviewed the methods used for the calculation of recombination coefficients, including some of the widely used semi-empirical formulae. Of all the atomic processes under consideration, the data for recombination are least reliable. Also, plasma properties such as density and potential may have significant influences on the rates. Dr Summers described the efforts being undertaken at JET to develop computer codes to evaluate recombination rates, and he agreed to lead efforts to recommend recombination data for Fe ions.

For plasma modelling the most commonly required ion-atom collision data are for electron capture from hydrogen by impurity ions. Dr Phaneuf reviewed the available data for ions of Fe colliding with atomic and molecular hydrogen. He found that, at least for high energies, almost all total electron capture data for partially-stripped Fe ions can be accurately represented by a single 8-parameter scaling curve. At low energies the database is rather sparse and the application of semi-empirical scaling formulae is rather dangerous in view of the complicated nature of the charge exchange process in this region. However a scaling formula

was presented which should be accurate to within 30%, except for fully-stripped and nearly fully-stripped ions.

The final afternoon was taken up with a discussion of the preparation and publication of a report detailing the results of the meeting. The main conclusions and recommendations are outlined in the following section.

C. Conclusions and Recommendations

The participants agreed to prepare and submit for publication a report of the proceedings of the meeting, containing recommended data. An informal report will be prepared before September 1986 and circulated to participants of the AGM, members of the IFRC Subcommittee on A & M Data for Fusion, and members of the A & M Data Centre Network. It was agreed that the most appropriate medium for publication is the journal Nuclear Fusion. J.G. Hughes will be responsible for coordinating the preparation and publication of the report. Other responsibilities were assigned as follows :

Charge Exchange

R.A. Phaneuf will be responsible for this section of the report. Data should be parameterized and presented in a simple form, taking advantage of scaling laws where appropriate. Cross sections, rather than rates should be presented, over the energy range 1eV - 1keV. J.G. Hughes will send Dr Phaneuf details of work carried out at Queens University Belfast on the scaling of low energy charge exchange data. Dr Summers will also send details of work done at JET on charge exchange.

Electron Impact Ionization

Dr Pindzola will be responsible for this section of the report. In collaboration with Professor Kingston, he will estimate the contributions from excitation-autoionization. Dr Hughes will provide curve fits to the recommended data.

Recombination

Dr Summers will be responsible for this section of the report. He will give some consideration to the effects on recombination rates of the plasma density. Dr Kato will provide parameterized fits to the recommended data of Dr Summers. Dr Pindzola also agreed to collaborate on this section.

Electron Impact Excitation

Professor Kingston will be responsible for this section of the report. Data exists for almost all ions of Fe and Professor Kingston will provide recommendations with error estimates for each transition. Rate coefficients should be provided. Dr Kato will provide parameterized fits to the recommended data.

It was decided that the calculation of radiation loss coefficients was a major research project which was not feasible at present, given the limited extent of the database for Fe. Dr Harrison will provide an analysis of this problem as part of Professor Kingston's section.

APPENDIX I

List of Participants

H.W. Drawin	Centre d'Etude Nucleaires, France
G. Fussmann	Max Planck Institut fuer Plasmaphysik, FRG
T. Kato	Institute of Plasma Physics, Nagoya, Japan
T. Kawamura	Institute of Plasma Physics, Nagoya, Japan
A. Miyahara	Institute of Plasma Physics, Nagoya, Japan
M.F.A. Harrison	Culham Laboratory, UK
A.E. Kingston	The Queen's University of Belfast, UK
H.P. Summers	JET Joint Undertaking, Culham Laboratory, UK
D.H. Crandall	Department of Energy, Washington, USA
R.A. Hulse	Plasma Physics Laboratory, Princeton, USA
R.A. Phaneuf	Oak Ridge National Laboratory, USA
M.S. Pindzola	Auburn University, Alabama, USA
J. Wiley	University of Texas at Austin, USA
J.G. Hughes	IAEA, Vienna, Austria
A. Lorenz	IAEA, Vienna, Austria

In Attendance

V.I. Pistunovich	Kurchatov Institute, Moscow, USSR
A.S. Kukushkin	Kurchatov Institute, Moscow, USSR

APPENDIX II

Advisory Group Meeting on Atomic Data for Fusion Plasma Modelling

IAEA, Vienna, 18-20 September 1985

Adopted Agenda

Wednesday, 18 September 1985

Morning Session: Chairman: Dr. H.W. Drawin

9:30	Opening Speech by Prof. V.I. Ferronsky
	Preliminary remarks by Scientific Secretary
9:45	Introduction and Review of Atomic Data Requirements for Fusion Plasma Modelling - Dr. H.W. Drawin
10:30	Discussion
11:00	Coffee
11:30	Effects of the Accuracy of Atomic Data on Tokamak Impurity Transport Modelling - Drs. T. Kawamura, T. Ono, A. Miyahara
12:00	Impurity Experiments on the TEXT Tokamak - Dr. J. Wiley

Afternoon Session: Chairman: Dr. D.H. Crandall

14:00	X-Ray and VUV Spectroscopy of the JIPPT-IIU Tokamak Plasmas - Drs. T. Kato, S. Marita, K. Masai
14:30	Joint Session with INTOR Specialists
16:00	Review of Electron Impact Excitation Data - Prof. A.E. Kingston

Thursday, 19 September 1985

Morning Session: Chairman: Dr. M.F.A. Harrison

9:00	Multi-step Ionization and K-shell Ionization for Plasma Modelling in Tokamaks - Drs. T. Kato and T. Fujimoto
9:30	Review of Electron Impact Ionization Data - Dr. M.S. Pindzola

Afternoon Session: Chairman: Prof. A. Miyahara

14:00 The Importance of Accurate Ionization and Recombination Rate Data for the Analysis of Tokamak Impurity Transport Experiments
- Dr. R.A. Hulse

14:30 Review of Electron-Ion Recombination Data
- Dr H.P. Summers

Friday, 20 September 1985

Morning Session: Chairman: Dr. D.H. Crandall

9:00 Measurement of Charge Exchange Recombination Lines on ASDEX
- Dr. G. Fussmann

9:30 Review of Charge Exchange Data
- Dr. R.A. Phaneuf

Afternoon Session: Chairman: Dr. H.W. Drawin

14:00 General Discussion, conclusions and recommendations

APPENDIX III

List of Papers Presented

[1] Electron Impact Ionization Data for the Fe Isonuclear Sequence.
M.S. Pindzola, D.C. Griffin, and C. Bottcher

[2] A Review of Electron-Ion Recombination with Emphasis on Ions of Fe.
H.P. Summers

[3] Charge Exchange Processes involving Iron Ions.
R.A. Phaneuf

[4] Electron Excitation.
A.E. Kingston

[5] Multistep Ionization and K-shell Ionization for Plasma Modelling of Tokamaks.
T. Kato and T. Fujimoto

[5] Effects of the Accuracy of Atomic Data on Tokamak Impurity Transport Modelling.
T. Kawamura, T. Ono, and A. Miyahara

[6] Impurity Transport at the University of Texas at Austin.
J. Wiley

[7] A & M Data for Fe - Data Available and Data Needed.
T. Tawara

[8] Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions: Flourine to Nickel.
M.A. Lennon, K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray, and F.J. Smith

[9] X-ray and VUV Spectroscopy of the JIPPT-IIU Tokamak Plasma.
T. Kato, S. Marita, and K. Masai

[10] Graphs Generated from the IAEA A & M EXFOR Numerical Database:
(a) Charge Transfer in Collisions of H Atoms with Fe Ions;
(b) Electron Impact Excitation of Fe Ions;
(c) Electron Impact Ionization of Fe Ions.
J.G. Hughes