XA9743326

International Atomic Energy Agency

INDC(NDS)-348

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Consultants' Meeting on

ELECTRON-IMPACT EXCITATION CROSS SECTION DATA FOR HELIUM

20 - 21 November 1995
Vienna, Austria

SUMMARY REPORT

K. Bartschat, I. Bray, F.J. de Heer, W.C. Fon, R.K. Janev

December 1995

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

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Printed by the IAEA in Austria
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Abstract

Brief proceedings and a summary of the conclusions of the IAEA Consultants' Meeting on "Electron-Impact Excitation Cross Section Data for Helium", held on 20-21 November 1995, in the IAEA Headquarters in Vienna, Austria, are provided. The main emphasis in the database analysis is given to the transitions between the states with principal quantum numbers n=2-4. The most important gaps in the existing database for these transitions have been identified, as well as the recently developed theoretical methods which can generate highly accurate cross sections. A course of action has been suggested for completing the electron-impact excitation database for helium in a timeframe conformal with the needs of present fusion energy research.

December 1995

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1. Introduction

The IAEA Consultants' Meeting on "Electron-Impact Excitation Cross Section Data for Helium" was convened on 20-21 November 1995, at the IAEA Headquarters in Vienna, Austria, with the objectives to review and critically assess the existing database on the e-He excitation processes, identify its most important deficiencies and gaps, and analyze the possible ways and means of its improvement and completion. The meeting was attended by four prominent experts in the field (see Appendix 1), three theoreticians and one experimentalist, and by part of the IAEA Atomic and Molecular Data Unit staff.

The organization of this IAEA consultancy meeting was in line with the Agency's effort to establish a complete and highly accurate cross section database for all processes involving helium (ground state and excited) atoms and the major fusion plasma constituents (electrons, protons and dominant impurity ions). The main applications of such a database in fusion energy research are the modeling of neutral helium beam attenuation in fusion plasmas and the transport of helium in fusion reactor divertors. Energetic (30-200 keV) neutral helium beams are introduced in fusion plasmas for diagnostic purposes and the attenuation of their intensity in the plasma is strongly affected by the plasma density and atomic processes of beam atoms with plasma particles. The beam intensity attenuation results from the loss of beam particles due to their ionization or charge exchange in collisions with plasma electrons and ions. When the neutral beam velocity is such that the collision times of excited beam atoms become comparable with (or longer than) their radiative lifetimes, multistep collision processes (such as excitation followed by ionization or charge exchange) begin to play an important role in the beam attenuation kinetics, resulting in a significant increase of the effective "beam stopping" cross section. The enhancement of beam attenuation at high beam energies is related with the increase of the population of excited states in the beam and the increase of electron removal cross section with increasing the excited state principal quantum number. At the considered collision energies, the excitation of the first few excited singlet states takes place much more effectively by heavy particle impact (protons, impurity ions) than by electrons. However, the excitation of higher excited states from the lower ones is more efficient by electron than by heavy-particle impact. Transitions between the states of different spin multiplicity (singlet-triplet and triplet-singlet transitions) are possible only by electron collisions. Therefore, the electron-impact transitions between the excited states of helium play a very important role in the beam attenuation kinetics.

The energy levels of the excited states of He with principal quantum numbers $n \geq 5$ can be considered degenerate and, consequently, the corresponding states can be regarded as hydrogen-like. For the transitions between the states with $n \geq 5$ one can use the hydrogenic approximations (e.g. for the electron wave function) or suitable cross section scaling relationships. The transitions between the states in the group with n=2-4, however, require to be treated individually.

The need of a radiative-collisional treatment of the kinetics of helium atoms in fusion reactor divertors stems not from the helium particle velocity but from the high electron plasma density in these regions. In this case, however, helium excitation from the ground state is also an important electron-impact process.

2. Meeting proceedings

At the beginning of the meeting, the Head of the IAEA Atomic and Molecular Data Unit reiterated the objectives of the meeting and then the Meeting Agenda (see Appendix 2) was discussed and adopted. The Agenda for the first working day included an analysis and critical assessment of the existing cross section data for electron-impact excitation of ground state and excited helium atoms. The discussions on the most critical gaps in the database and the existing computational capabilities for generation of the required data were left for discussion during the second day of the meeting.

Since the transitions from the ground state have been subject of a detailed analysis at a previous IAEA experts' meeting related to the "Helium Beam Fusion Alpha Particle Diagnostics" (June 1991) and its findings reported in Nuclear Fusion A+M Supplement vol. 3 (1992), the present consultancy meeting focused its work on the assessment of available cross sections for transitions from excited states, mainly within the group of states with principal quantum numbers n=2-4. A comprehensive compilation of all the existing theoretical and experimental (for a few transitions) data has been prepared and reported at the meeting by Dr. F.J. de Heer. This collection served as a basis for the data intercomparison and assessment analyses performed at the meeting. Prof. K. Bartschat reviewed the recent developments of the R-matrix method with inclusion of pseudo-states (RMPS-method) at the Queen's University of Belfast and reported on its first results. Prof. I. Bray described the basic features of the convergent close-coupling (CCC) method recently developed at the Flinders University of South Australia and reported the cross section results obtained by this method for many transitions from the $2^{1,3}S$ states of helium. Prof. W.C. Fon provided extensive comments on the standard R-matrix method, its various features and limits of applicability.

The analysis of database completeness for the transitions with the n=2-4 group of states revealed that for the transitions from $2^{1,3}S$ the available cross section information is, generally speaking, adequate (with the exception of a few cases), but for the transitions from $2^{1,3}P$ and $n^{1,3}L$ (n=3,4; L=S,P,D) the cross section information is either absent or of, generally, very low accuracy. The recently developed CCC and RMPS codes have been identified as currently the most powerful available theoretical tools for generation of the missing (or of inadequate accuracy) excitation cross section data. Details of the findings of the meeting regarding the data status and the ways of its possible improvements are given in the following sections of this Report.

3. Status of e-He excitation database

3.1 Excitation from the ground state of He

The experimental data for electron impact excitation of He(1^1S) to He($n^{1,3}L$), n=2-6, have been recently critically reviewed (F.J. de Heer et. al., Supplement to the Journal Nuclear Fusion 3 (1992) 7). A preferred data set is now being established and combined with theoretical close-coupling approximation data below the ionization threshold and Born approximation data at high energy. The experimental data are between 30 and 2000eV electron impact energy for singlet excitation merging well with the theoretical Born data, and up to less high impact energy for triplet excitation (because the cross section becomes very small with increasing energy, as it follows from the Ochkur approximation). Below 30eV an extrapolation is made towards the close-coupling (29-states R-matrix) calculations from threshold up to the ionization energy (Berrington et. al., personal communication). Except for the metastable 2^1S and 2^3S states, most experimental data are from photon emission cross section measurements. For metastables the (integrated) cross sections have been obtained by using angular differential inelastic (energy loss selected) scattering cross sections.

The errors are, generally, smallest for singlet states (optical measurements) above about 40eV, i.e. $\leq 10\%$ and the recommended R-matrix and Born data are accurate to better than 10% and 5%, respectively. At low energies (< 40eV) errors in experiment may increase up to about 30%.

Errors in experimental triplet cross sections (optical data) are relatively large, in particular at high energies, because secondary effects, such as collision transfer, are difficult