International Atomic Energy Agency

INDC(NDS)-292

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

# 1st IAEA Research Co-ordination Meeting on "Atomic Data for Medium- and High-Z impurities in Fusion Plasmas"

22-24 September 1993, Vienna Austria

## SUMMARY REPORT

Prepared by R.K. Janev

January 1994

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

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## Abstract

The proceedings of the 1st IAEA Research Co-ordination Meeting on "Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas" (September 22-24, 1993, Vienna, Austria) is briefly described. The Data Status Report, prepared by the meeting participants, along with the Meeting conclusions and recommendations, is reproduced. The progress reports on the work performed within the individual research projects of this CRP are also included in this Summary Report.

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January 1994
94-00409

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## 1. INTRODUCTION

The 1st Research Co-ordination Meeting (RCM) of the IAEA Co-ordinated Research Programme (CRP) on "Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas" was convened on September 22-24, 1993, at the IAEA Headquarters in Vienna. The objectives of the meeting were to review the work accomplished within the Programme during the last two years and co-ordinate the research efforts for the remaining period of the CRP. The Meeting was attended by seven (out of ten) representatives of the individual projects within the CRP, and by Drs. V.A. Abramov (Kurchatov Institute, Moscow), W.L. Wiese (NIST, Gaithersburg) and H. Tawara (NIFS, Nagoya) as observers. Drs. R. Morgenstern (KVI, Groningen), A. Müller (Univ. of Stuttgart) and V. Zoran (IAP, Bucharest), participants of this CRP, were not able to attend the meeting. The list of meeting participants is given in Appendix 1.

## 2. BRIEF MEETING PROCEEDINGS

After the adoption of Meeting agenda (see Appendix 2), the work of the meeting proceeded in the following sessions:

1) Electron-ion/atom collisions,
2) Heavy particle collisions,
3) Assessment of data status and work co-ordination,
4) Meeting conclusions and recommendations.

Below we give the highlights of meeting presentations and discussions.

In the session on electron-ion collision processes, Dr. P. Defrance (Catholic University of Louvain) reported experimental (crossed beams) cross section results on the single and double ionization of $Ne^{q+}$, $Ar^{q+}$ and $Kr^{q+}$ ions by electron impact in the energy range from 20 eV to 6 keV. The charge states investigated were: $Ne^{6,8+}$ for single ionization (SI), $Ne^{5,6+}$ for double ionization (DI), $Ar^{8,10+}$ for SI, $Ar^{7-10+}$ for DI, $Kr^{8,18+}$ for SI and $Kr^{7,8+}$ for DI. For most of these ions, the corresponding cross section data have been obtained for the first time. The group of Dr. Defrance is planning to continue these measurements and provide systematic SI and DI cross sections for all $Kr^{q+}$ ions with q=8-18. Extension of these measurements to metallic ions is also planned in the near future.

Dr. V.P. Shevelko (Lebedev Physical Institute, Moscow) presented extensive CBE calculations of electron impact direct ionization cross sections for ions in ground and excited states ($n\ell$=1s-6h). Simple analytic fits to these cross sections, as well as to their Maxwellian averages, were also presented. The l-averaged cross sections have also been fitted to analytic expressions, the fitting parameters of which turned out to be smooth functions of n allowing extrapolation of the fitting formulae to ionization from $n \geq 7$ states. The claimed validity of the obtained fits is $E < 15I$ for the cross sections, and $0.1I \leq T \leq 8I$ for the reaction rate coefficients, where I is the binding energy of the valence electron.

Dr. C.C. Havener (ORNL, Oak Ridge) provided a detailed report on the experimental work done at ORNL on electron-ion, ion-atom collisions, ion-ion (and ion-surface) collisions. New electron-ion cross section data for the single ionization in $e + Si^{+}$, $Si^{2+}$, $Si^{6,7+}$ and $Kr^{4,5,7+}$ were presented. The results for the electron-impact 3s-3p excitation of $Si^{3+}$ and $4s^2\,{}^1S \rightarrow 4s\,4p\,{}^3P$ intercombination transition in $Kr^{6+}$ were also shown. The results of the first merged-beams measurements of electron capture cross sections for $Si^{4+}$ collisions with ground and excited state hydrogen atoms were reported. The preparatory work for merged-beams electron capture cross section measurements in ion-ion ($Ar^{5+} + Ar^{6+}$) collisions was described. In addition to this, Dr. Havener presented also the results of recent work at ORNL on ion-surface collisions (neutralization and relaxation processes of multicharged ions colliding with Be, Cu and Au single crystal surfaces).

In the second meeting session devoted to the processes in heavy-ion collision, Prof. H.B. Gilbody (Queen's University of Belfast) presented the recent results on electron capture and ionization of experimental studies performed by the QUB group for collisions of metallic ions atoms with hydrogen and helium atoms and ions. These studies include: state selective electron capture in collisions of $Fe^{3,4+}$ ions with H and He atoms (using the method of translational energy spectroscopy), electron capture, ionization and transfer ionization in collisions of protons and alpha particles with Mg, Fe and Cu atoms, and charge transfer and ionization in collisions of protons with $Al^{+}$, $Ga^{+}$, $In^{+}$ and $Tl^{+}$ ions. These studies have revealed the important role of the transfer ionization channel in the charge changing collisions of the investigated collision systems. Prof. Gilbody also reported electron-impact multiple ionization cross sections for Mg, Fe and Cu atoms in a wide energy range.

Dr. W. Fritsch (HMI, Berlin) reported on the recent important developments in the application of semi-classical close-coupling method to the charge transfer processes involving many electron ions and/or targets and to the description of low-energy excitation in one-electron systems. A particularly important achievement of this effort is the description of one-electron transfer from hydrogen molecules. The specific collision systems, for which electron capture studies have been performed during the reporting period, include: $H^+$, $He^{2+}$, $C^{4+}$, $Ti^{4+}$, $Fe^{8+} + H_2$, $Ti^{4+}$ + He, and $Ni^{10+}$ + H. The low-energy excitation studies include the systems $Z^{Z+} + H$ ($Z \leq 6$) with a record number of atomic (and pseudo-) states in the basis (e.g. over 200 for Z=6). These latter studies provide also highly accurate cross sections for the state selective electron capture channels.

Dr. K. Katsonis (LPGP, Orsay) presented a comprehensive set of electron capture and ionization cross sections obtained by the Classical Trajectory Monte Carlo (CTMC) method in a broad energy range. The systems studies include: $A^{q+}$ + H, $q \leq Z$ ($\leq 75$) (q=3-8 for the shell-selective electron capture), $A^{q+}$ + He ($q \equiv Z = 1\text{-}28$), and $A^{q+} + He^+$ ($q \equiv Z=1\text{-}18$). In the case of He target, the cross sections for two-electron processes have also been calculated in this study.

Dr. H. Tawara (NIFS, Nagoya) presented considerations regarding the possible role of stripping reactions during the energetic neutral hydrogen beam penetration in the peripheral region of fusion plasmas. If proven important, this process would increase the effective ion charge of the boundary plasma.

Dr. C. Cisneros (Laboratorio de Guernavaca) presented an exhaustive compilation and evaluation of the existing experimental and theoretical cross sections for total electron capture of Si, Ni, Ti, Mo and W ions colliding with H, $H_2$ and He. The compilation and their analysis includes all the literature data as of December 1992. the methods and the criteria applied in the data accuracy assessment were also presented.

Dr. R.K. Janev (IAEA) presented the results of low-energy ionization calculations by the adiabatic superpromotion (hidden crossings) model for $He^{2+}$, $C^{6+}$, $O^{8+}$ + H and showed a cross sections scaling relationship following from the model and confirmed by the numerical calculations. He also showed that the excitation cross sections for the $n^1L$ term series of He by proton and multicharged ion impact exhibit distinct scaling properties with respect to the binding energy and the ionic charge state (as well as the oscillator strength for L=P).

The third session of the Meeting was devoted to a thorough analysis of the status of the presently available database for the collision processes involving medium- and high-Z plasma impurities (having particularly in mind the needs of current and near-future fusion research), assessment of the overall contribution of the present CRP to the improvement of this database, and the prospects (and associated problems) for generating a reasonably complete collisional database for the most important medium- and high-Z plasma impurities. The findings of this analysis are given in the next three sections of the present report.

## 3. DATA STATUS REPORT

## (Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas)

H.B. Gilbody (Chairman), J. Botero, C. Cisneros, P. Defrance, W. Fritsch, C.C. Havener, R.K. Janev, K. Katsonis, V.P. Shevelko and H. Tawara

### 1. Introduction

In previous advisory meetings [1,2] of the IAEA, atomic and molecular data on fusion impurities including some medium- and high-Z species have been considered. A recent IAEA report [3] has emphasized the need for data on medium- and high-Z species in the context of the plasma edge and central plasma parameters of ITER. There is a need for data for diagnostics based on charge exchange emission spectroscopy, beam emission spectroscopy and alpha particle diagnostics.

In this meeting, recent data on the medium-Z impurities Al, Si, Ti, V, Cr, Fe, Ni, Cu and Ga and high-Z impurities Mo, Ta and W have been considered. Data on Kr are also relevant to proposed plasma diagnostics in ITER. Apart from recently published data, some measurements and calculations have been carried out as part of the IAEA Co-ordinated Research Programme and presented at this meeting.

In some areas, particularly those concerned with high-Z species, further experimental and theoretical studies of impurity processes seem likely to be limited by the scarcity of many spectroscopic data, energy levels, transition probabilities and excited state lifetimes.

### 2. Electron collision processes

The main processes of interest are:

$e + X \rightarrow X^+$ ionization

and

$e + X^{q+}$ collisions involving ionization, excitation and recombination.

#### (i) Electron impact ionization of atoms

Measurements are not available for all species and there are large discrepancies between many existing data. The measurements based on the fast crossed beam technique by Freund et al [4] include single ionization cross sections for Fe, Cu, Al and Kr. The data for Al and Kr are believed to be accurate to within ± 10% but the Fe and Cu data are much less reliable. New measurements for Fe and Cu based on a crossed beam technique using thermal energy ground state atoms presented at this meeting by Shah et al [5] and by Bolorizadeh et al [6] provide data over an extended energy range for both single and multiple ionization. These new measurements, in particular, are believed to provide cross sections of improved accuracy for single ionization.

(ii) Electron impact ionization of ions

Compilations of recommended data for Fluorine to Nickel by Lennon et al [7] published in 1986 and for Copper to Uranium by Higgins et al [8] published in 1989 are available. A bibliography by Itikawa [9] covers ionization data published during the period 1983-1989 and a summary of available data is also provided in the 1991 IAEA report [2]. Data for medium-Z ions not included in the latter report includes measurements for single ionization of $Al^{2+}$ and $Si^{3+}$ by Crandall et al [10], $Si^{+}$ and $Si^{2+}$ by Djuric et al [11], $Si^{4+}$ and $Si^{5+}$ by Thompson et al [12], $Si^{6+}$ and $Si^{7+}$ by Zeijlmans et al [13], $Fe^{6+}$ by Gregory et al [14], $Ga^{2+}$ and $Ga^{3+}$ by Belyaev [15], $Ta^{3+}$ and $Ta^{8+}$ by Gregory et al [16], $Kr^{2,3,4,7,8,9+}$ by Gregory and Bannister [17], and $Kr^{1,2,3+}$ by Tinschert et al [18]. Cross sections for double ionization are much smaller than those for single ionization. Double ionization cross sections for $Kr^{1,2,3,4+}$ have been measured by Tinschert et al [18], and for $Kr^{8+}$ by Qualin and Defrance [19] reported at this meeting.*

Shevelko [20] has reported at this meeting theoretical estimates of cross sections and rate coefficients for direct ionization of multicharged ions in ground or excited states including ionization of inner shell electrons. The calculations are believed to be valid up to impact energies 15 x Binding Energy of the target electron shell.

(iii) Electron impact excitation of ions

Electron impact excitation data are included in the review by Itikawa [9]. A more recent compilation is given by Pradhan and Gallagher [21]. Since the IAEA report [2] some data for medium-Z ions have become available. These include measurements for

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* Storage ring experiments on single ionization of $Cl^{14+}$ and $Fe^{15+}$ have been performed in Heidelberg (see the Progress Report of Prof. A. Müller in Appendix 3).

$Si^{3+}$ by Wahlin et al [22] for $Kr^{6+}$ by Bannister et al [23] and for $Si^{11+}$ by Konig et al[24]. Measurements for highly charged ions based on the use of EBIT have been carried out by Wong et al [25] in the case of $Ti^{19+}$ and $Ti^{20+}$, $V^{21+}$, $Cr^{21+}$ and $Cr^{22+}$, $Mn^{22+}$, $Mn^{23+}$, $Fe^{23+}$ and $Fe^{24+}$.

Calculations for the resonant excitation processes based on the R-matrix approach have been considered in a publication edited by Burke and Berrington [26]. Shevelko [27] has presented analytic formulae for dipole excitation cross sections and rates.

(iv) Recombinations

Radiative recombination, dielectronic recombination and three-body recombinations are processes which are all relevant to fusion data requirements. Radiative recombination is considered in a recent review by Pajek and Schuch [28], and previously by Hahn [29] for Ti, Cr, Fe and Ni ions.

The dielectronic recombination process $e + X^{q+} \rightarrow X^{(q-1)+**} \rightarrow X^{(q-1)+*}$ is of considerable importance for medium- and high-Z ions. Recent data have been given within the reviews by Hahn [29], Dunn [30] and in the publication edited by Graham et al [31]. Some measurements have recently been carried out for $Cu^{26+}$ by Kilgus et al [32].

## 3. Heavy particle collision processes

Collision processes involving, H, He and $H_2$ are of primary concern. The energy range of interest extends from ~ eV to MeV.

At low energies, plasma edge densities are such that ion-atom interchange processes in $H_2$ should be considered. Experimental data on such processes have been reviewed by Armentrout [33] for ions of the transition elements and of Si and Kr.

Electron capture, ionization and excitation in collisions of $X^{q+}$ ions with H, He and $H_2$ are of considerable importance and data are required over a wide energy range for all charge states q. For H and He there is a need for data on excited as well as for ground state atoms.

(i) Total cross sections for electron capture

A review of the experimental and theoretical total cross sections for one-electron capture by singly and multiply charged ions of Si, Ti, Ni, Mo and W in collisions with H, $H_2$ and He has been given by Cisneros et al [34] at this meeting. Other reviews have been given by Wu et al [35] and by Tawara [36]. The accuracy of many of the experimental cross sections particularly at low impact energies is subject to large uncertainties arising from unknown fractions of metastable species in the primary ion beams. There are no data for two-electron capture and for transfer ionization in $H_2$ and He.

At high velocities v ≥ a.u. and for $q \geq 3$ general scaling procedures [37,38] may be used to predict cross sections for one-electron capture in H, $H_2$ and He with an accuracy generally within 50%. At lower impact energies, scaling procedures are less appropriate. At this meeting Katsonis [39] has presented calculations based on the classical-trajectory Monte-Carlo (CTMC) method which predict cross sections for one-electron capture which should be valid for $q \geq 4$ in the ranges 1-600 keV $u^{-1}$ for H and He respectively.

New experimental data [40] for electron capture in $Si^{4+}$ - H collisions in the range 1-1000 eV $u^{-1}$ were presented at this meeting.

(ii) Cross sections for state-selective electron capture

Experimental measurements are very limited. Cross sections for one electron capture by $Al^{2+}$ ions in H and $H_2$ and keV energies are available [41]. Measurements based on translational energy spectroscopy presented at this meeting [42,43] for $Fe^{3+}$ and $Fe^{4+}$ in H and He identify the main excited product states but a detailed analysis of the data is precluded by the presence of unknown fractions at metastable ions in the primary beams. Future experimental and theoretical work will be limited by the lack of many basic spectroscopic data for high Z ions including energy levels and transition probabilities/lifetimes. It is important that future experimental measurements should be carried out, where possible, with primary beams in well defined ground or specified excited states.

At this meeting Fritsch [44] described close coupling calculations for state-selective electron capture for $Ti^{4+}$ + He, $H_2$, $Fe^{8+}$ + $H_2$ and $Ni^{10+}$ + H which are expected to be valid in the range 1-100 eV $u^{-1}$. These complement the earlier calculations of Fritsch [45] for the $Ti^{4+}$, $Cr^{6+}$ and $Fe^{8+}$ - H collision systems. Earlier calculations by Fritsch and Tawara [46] provide data for $Si^{4-14+}$ + H collisions. The CTMC calculations by Katsonis [39] presented at this meeting also provide predictions of state-selective electron capture for $q \geq 4$ at moderate velocities.

(iii) Cross sections for ionization

Cross sections for ionization of H, $H_2$ and He for the species primary of interest are extremely limited and have been described in an earlier IAEA report [1]. At high energies (above about 200 keV $u^{-1}$) cross sections are q rather than species dependent and increase according to $q^n$ where n varies slowly with velocity. The scaling relations given by Gillespie [47] can be used for ions with $q \geq Z/2$ to predict cross sections in H, $H_2$ and He with reasonable accuracy for $(E/A)/q \geq 30$ keV $u^{-1}$. Additional data and a low-energy scaling of ionization cross sections were presented by Janev [48] at this meeting.

Some measurements of cross sections for single and double ionization of helium by fast highly charged projectiles have been carried out by Berg et al [49].

(iv) Cross sections for excitation

Experimental measurements of excitation of H, $H_2$ and He by medium- and high-Z ions are very limited. There are some recent experimental measurements in He by Anton et al [50] for the excitation of $n^1P$, $n^1S$ and $n^1D$ states of He for $q \geq 1$ which are believed to be valid over a wide energy range. Janev [48] has showed at this meeting that the data for each term series can be scaled with respect to the transition energy (and the oscilator strength for the $n^1P$ excitation).

For excitation of hydrogen atoms by multiply charged ions the cross section can be obtained by q scaling of the Lodge et al [51] formula for proton impact excitation. Cross section calculations for ions with q=2,6,8 and 26 on H(n) atoms with n=1,2,3,4, $\Delta n$=1,2,3 performed by Rheinhold et al [52] in the symmetric eikonal approximation and further supported by the results of the CTMC method, show that this scaling procedure is justified down to reduced energies of about 15 keV $u^{-1}q^{-1}$.

At lower reduced energies, the calculated excitation cross sections for bare charges q=1-6 [53] provide some guidence for assessing excitation by q-charged projectiles which have not been studied so far.

5. Collisions involving excited H atoms

Although there are no data for medium and high Z primary ions, crossed beam studies by Kim and Meyer [54] provide total cross sections for electron removal from highly excited H(n=9-24) atoms in collisions with $N^{(1-5)+}$, $O^{(1-5)+}$ and $Ar^{(1-5)+}$ ions at velocities in the range 1-2 a.u. where ionization is dominant. Measured cross sections for different H(n) populations (selected by electric field ionization) for a given q and v are independent of species and increase with $q^2$. Detailed studies of the n dependence were precluded by the presence of the electric field in the collision region. New merged beam measurements [40] which extend down to very low energies ~ 0.1eV $u^{-1}$ where electron capture is dominant indicate that cross sections can be described by the $n^{-4}$ scaling. At velocities $v > 1$ a.u. electron capture cross sections are expected to scale accordingly to $n^{-3}$. A double-scaling (in both q and n) formula for the total electron capture cross sections from excited (hydrogen-like) states, covering both the low and high collision energies, has recently been derived by Janev [55].

(vi) Ion-ion collisions

Cross sections for charge transfer,

$H^+ + X^+ \rightarrow H(\Sigma) + X^{2+}$

where $H(\Sigma)$ denotes all final bound states, and ionization

$H^+ + X^+ \rightarrow H^+ + X^{2+} + e$

have been measured by Watts et al [56] for $Al^+$, $Ga^+$, $In^+$ and $Ti^+$ ion for C.M. energies in the range 50-597 keV. At these energies $X^{2+}$ production is dominated by the ionization process. A recent study by Murphy et al [57] of $Tl^{3+}$ production in $H^+$ - $Tl^+$ collisions indicates that the transfer ionization process

$H^+ + Tl^+ \rightarrow H + Tl^{3+} + e$

is dominant $Tl^{3+}$ production process at the lower collision energies considered.

Measurements and calculations for collision processes between multiply charged ions are extremely limited. A folded-beam ion-ion collision experiment has been described by Kim and Janev [58] to study $X^{4+}$ formation in $X^{3+}$ collisions for X = Ar or Kr at a C.M. energy of 60 keV. Measured cross-sections of about 6.1 x $10^{-16}$ $cm^2$ and 2.9 x $10^{-16}$ $cm^2$ for Ar and Kr ions respectively are quite large.

Studies of excitation in ion-ion collisions are also very limited. Scheibner et al [59] have calculated cross sections for $2^2S_{1/2}$ - $2^2P_{1/2,3/2}$ transitions in collisions between protons and hydrogen-like He, Ne, Ar and Fe in the range 27-2700 eV.

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## 4. SUMMARY OF CRP ACCOMPLISHMENTS

During the last two years, the participants of the present CRP generated a substantional amount of new cross section information regarding the processes of intermediate-to-high-Z plasma impurity ions. The CRP effort was focussed on the intermediate-Z ions Al, Si, Ti, Cr, Fe, Ni and Cu with somewhat less attention to the high-Z ions of relevance to fusion, (such as Mo, W, Ta), due to the lack of basic spectroscopic information for the latter. Extensive studies within the present CRP have been performed for all processes involving noble gas atoms and ions (Ne, Ar, Kr) which are important for fusion plasma diagnostics and, possibly, for plasma burn control. Compilation and critical assessment of the available cross section information for the collision processes of medium-to-high-Z plasma impurities with the basic plasma constituents ($e^-$, H, $H_2$, He and their ions) was also a significant outcome of the present joint effort. Probably the most important result of the present CRP is the generation of scientific interest in the atomic physics community for these collision systems which can produce beneficial long-term effects on the data generation for these systems. During the period of this CRP a number of experimental facilities have been constructed (also outside the present CRP) for studying the collision processes of metallic ions. On the theoretical side, methodological developments have been undertaken to more adequately describe the interaction potentials and collision dynamics of many electron collision systems at low and intermediate energies. The awareness of the insufficient, but required, spectroscopic information for high-Z ions and of the role of metastable beam fractions in beam-beam coincidence experiments have greatly increased. Expressed in quantitative form, the major achievements of the present CRP can be summarized as:

(1) Publication of a compendium of data on "Collision processes of metallic impurities in fusion plasmas" (Physica Scripta T37, 1991);

(2) Publication of more than 15 critical reviews and data status and quality assessments for specific classes of collision processes involving the considered types of plasma impurities;

(3) Publication of more than 90 scientific articles in recognized international journals on the processes studied within the present CRP;

(4) A comprehensive compilation and assessment of available electron capture cross section data for the Si, Ti, Ni, Mo and W ions colliding with H, $H_2$ and He (C. Cisneros);

(5) Generation and ALADDIN formatting of a large set of systematic CTMC cross section data for electron capture and ionization in collisions of multicharged ions with H, $He^+$ and He.

## 5. MEETING CONCLUSIONS AND RECOMMENDATIONS

1) Despite of the growing interest of atomic physics community in generating cross section data for the collision processes of medium- and high-Z fusion plasma impurities, the available database is still far from completion and from satisfying the needs of current fusion programme, including the design of ITER.
2) The most important gaps in the considered database are for the high-Z elements of interest (Kr, Mo, W) where even the spectroscopic information is not available.
3) The present CRP has provided a significant direct contribution to the collisional database of considered plasma impurities and stimulated a general scientific interest in the atomic physics community for the studies of these collision systems.
4) In view of broad range of species and processes involved, the Meeting participants suggest a selective approach in filling the gaps in the high-Z collisional database through organized international efforts. The Agency is particularly encouraged to undertake appropriate actions on generation of the spectroscopic and collisional databases for Kr, Mo and W.
5) The present CRP will continue its work on data compilation and generation during 1994, with emphasis on the high-Z plasma impurities. The experimental facilities developed at some laboratories during the previous two years are expected to generate a significant amount of cross section information in 1994 and 1995.
6) The Meeting participants agreed that the results of the present CRP, presented in an appropriate form, be published as a topical issue of Physica Scripta, if that would be acceptable for the journal.

# Appendix 1

## 1st IAEA Research Co-ordination Meeting on "Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas"

**22-24 September 1993, Vienna, Austria**

## LIST OF PARTICIPANTS

| | |
|---|---|
| Dr. P. Defrance | Université Catholique de Louvain, Dept. de Physique, FYAM, Chemin du Cyclotron 2, B-1348 Louvain-la-Neuve, BELGIUM |
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# Appendix 2

## 1st IAEA Research Co-ordination Meeting on "Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas"

**22-24 September 1993, Vienna, Austria**

**MEETING AGENDA**

Wednesday, September 22 Room: A-07-42

| | | |
|---|---|---|
| 09:30 - 09:45 | - Opening<br>- Adoption of Agenda | |
| **Session 1.** | Electron-Ion/Atom Collisions | |
| Chairman: | W. Fritsch | |
| 09:45 - 10:30 | P. Defrance: | Electron impact ionization of rare gas ions |
| 10:30 - 11:15 | V.P. Shevelko: | Electron impact ionization of high-Z ions in ground and excited states |
| 11:15 - 11:30 | **Coffee break** | |
| 11:30 - 12:15 | C.C. Havener: | Plasma impurity cross section data involving e-ion and ion-atom collisions at ORNL |
| 12:15 - 14:00 | **Lunch** | |
| **Session 2.** | Heavy Particle Collisions | |
| Chairman: | P. Defrance | |
| 14:00 - 14:45 | H.B. Gilbody: | Charge transfer and ionization studies involving metallic species |
| 14:45 - 15:15 | K. Katsonis: | Charge transfer and ionization in ion-atom collisions |
| 15:15 - 15:45 | H. Tawara: | Enhancement of the effective charge of impurity ions during neutral beam injection |
| 15:45 - 16:00 | **Coffee break** | |
| 16:00 - 16:45 | W. Fritsch: | Studies of selected medium-Z highly charged plasma impurity metallic ions with H and $H_2$ |
| 16:45 - 17:30 | C. Cisneros: | Experimental and theoretical cross section data for single electron capture in collisions of Si, Ti, Ni, Mo and W ions with H, $H_2$ and He |
| 17:30 - 18:00 | R.K. Janev: | On the scaling properties of excitation and ionization cross sections of H and He colliding with multiply charged ions |

Thursday, September 23

**Session 3.** Assessment of the data status for collision processes involving medium- and high-Z plasma impurities

Chairman and Co-ordinator: H.B. Gilbody

09:00 - 12:00 The work of this meeting session should include the following:

1) Analysis of the existing database vs. fusion research data needs;
2) Assessment of the contribution of present CRP to the plasma impurity collisional database (summary of CRP accomplishments to-date);
3) Possible co-ordination of future work plans within the CRP;
4) Assessment of prospects and time-scale for establishing a complete "core" collisional database for metallic plasma impurities;
5) Preparation of a report on the data status and the CRP accomplishments.

12:00 - 14:00 **Lunch**

14:00 - 18:00 **Session 3.** (Continues)

Friday, September 24

| | |
|---|---|
| **Session 3.** | (Cont'd.) |
| 09:00 - 12:00 | - Prepartation of data status report (cont'd.);<br>- Forumulation of a brief summary of meeting conclusions and recommendations. |
| 12:00 - 14:00 | **Lunch** |
| **Session 4.** | Meeting Conclusions and Recommendations |
| Chairman: | R.K. Janev |
| 14:00 - 15:00 | Discussion and adoption of Meeting conclusions and recommendations |
| 15:00 - 17:00 | Disscusion of the final CRP document (content, contributors, publication) |
| **17:00 -** | **Adjourn of the Meeting** |

Appendix 3

# PROGRESS REPORTS OF INDIVIDUAL CRP PROJECTS

# IAEA Coordinated Research Programme on Atomic Data for Medium and High Z Impurities in Fusion Plasmas

## IAEA Research Agreement No. 6721/CF

## Charge transfer and ionization studies involving metallic species

**Progress report by** **Professor H B Gilbody**
**Department of Pure and Applied Physics**
**The Queen's University of Belfast**

The programme has involved the following experimental investigations:-

### 1. State selective electron capture in collisions of slow $Fe^{3+}$ and $Fe^{4+}$ ions with H and He atoms.

Translational energy spectroscopy (TES) using primary $Fe^{q+}$ ions from an ECR ion source has been used [1] to study the following processes

$$Fe^{q+} + H \rightarrow Fe^{(q-1)+}(n,l) + H^+$$

and $Fe^{q+} + He \rightarrow Fe^{(q-1)+}(n,l) + He^+(n', l')$

for q = 3 and 4 at energies of q x 2 and q x 3 keV. With the exception of a TES study [2] of one-electron capture by $Al^{2+}$ in H and $H_2$ our earlier work, carried out without an ECR source, has been able to address only processes involving non-metallic primary ions.

The main excited products are shown to arise through electron capture into n=3 and n=4 states of the $Fe^{(q-1)+}$ ions. Electron capture by $Fe^{3+}$ ions is shown to be dominated by many collision product channels involving metastable ions present in the primary beams. Since the metastable fractions and lifetimes of the relevant states are unknown a detailed analysis is precluded. The dominant role of metastable primary ions indicates that previously published total electron capture cross sections for $Fe^{3+}$ ions require cautious interpretation.

In the case of $Fe^{4+}$ impact, the observed energy change spectra can be satisfactorily interpreted in terms of a dominant contribution from collision channels involving ground state primary ions. We have also carried out multi-channel Landau-Zener calculations for both H and He targets which satisfactorily describe only the main observed collision product channels.

In future work double translational spectroscopy will be used to try to obtain data for primary ions in either ground or selected metastable states.

## 2. Electron capture and ionization in collisions of fast $H^+$ and $He^{2+}$ ions with Mg, Fe and Cu atoms

A crossed beam technique incorporating time-of-flight spectroscopy and coincidence counting of fast ion-slow ion collision products has been used to obtain individual cross sections ${}_{z0}\sigma_{mn}$ for electron capture, transfer ionization and pure ionization in processes

$X^{z+} + Y \rightarrow X^{m+} + Y^{n+} + (m+n-z)e$ where m and n are specified. Data have been obtained for primary ions $H^+$ and $He^{2+}$ and target atoms Mg, Fe and Cu.

In the case of Mg results [3] for one and two-electron capture in processes involving $Mg^{n+}$ formation for n=1-4 have been obtained for 90-2000 keV $u^{-1}$ $H^+$ impact and 43-500 keV $u^{-1}$ $He^{2+}$ impact. At these energies, in addition to the outer 3s electron, the inner 2s and 2p electrons in Mg are expected to become important. While $Mg^+$ production is dominated by pure ionization in the energy range considered, the important role of transfer ionization in the formation of $Mg^{2+}$, $Mg^{3+}$ and $Mg^{4+}$ ions has been clearly demonstrated. Transfer ionization rather than simple charge transfer has been shown to provide the dominant contributions to one-electron capture by $H^+$ and to both one and two-electron capture by $He^{2+}$ ions. Some discrepancies in magnitude with previously published low energy data [4] are believed to reflect, in part, the use of different calibration procedures.

In the case of Fe, measurements of one electron capture by $He^{2+}$ ions have been carried out [5] in the range 70-500 keV $u^{-1}$ for $Fe^{n+}$ production where n = 1-6. For $H^+$ impact cross sections ${}_{10}\sigma_{0n}$ decrease with increasing energy. Above 250 keV $u^{-1}$ cross sections ${}_{10}\sigma_{02}$ exceed ${}_{10}\sigma_{01}$. For $He^{2+}$ impact, transfer ionization cross sections, ${}_{10}\sigma_{12}$, ${}_{10}\sigma_{13}$ and ${}_{10}\sigma_{14}$ all exceed ${}_{10}\sigma_{11}$ at the higher impact energies. In the case of two-electron capture by $He^{2+}$ ions cross sections ${}_{20}\sigma_{03}$ and ${}_{20}\sigma_{04}$ provide the dominant contributions.

Preliminary results only are available [5] for Cu for processes where n = 1-6 and these also demonstrate the importance of transfer ionization processes.

## 3. Charge transfer and ionization in collisions of protons with $Al^+$, $Ga^+$, $In^+$ and $Tl^+$ ions

In earlier work [6] we used a fast intersecting beam technique to obtain cross sections $\sigma_c$ for charge transfer

$$H^+ + X^+ \rightarrow H(\Sigma) + X^{2+}$$

and $\sigma_i$ for ionization

$$H^+ + X^+ \rightarrow H^+ + X^{2+} + e$$

together with total cross sections $\sigma(X^{2+}) = (\sigma_c + \sigma_i)$ for $Al^+$, $Ga^+$, $In^+$ and $Tl^+$ at c.m. energies in the range 50-597 keV. Ionization cross sections $\sigma_i$ were shown to provide the main contribution to $\sigma(X^{2+})$ at the energies considered. A simple classical scaling relation has been shown to allow predictions in agreement to within a factor of two of high energy values of $\sigma_i$.

In our recent work [6], $Tl^{3+}$ production in $H^+$-$Tl^+$ collisions has been studied in the c.m. energy range 80-299 keV. Transfer ionization is shown to be more important than direct ionization in $Tl^{3+}$ production at the lower impact energies.

## 4. Multiple ionization of Mg, Fe and Cu by electron impact

A pulsed crossed beam technique incorporating time-of-flight spectroscopy is being used with a specially developed thermal energy beam of metallic atoms to obtain cross sections for multiple ionization processes

$$e + X \rightarrow e + X^{n+} + ne$$

over a wide energy range. Cross sections $\sigma_n$ for the formation of 1-4 times ionized Mg, 1-4 times ionized Fe and 1-5 ionized Cu have been obtained in the respective energy ranges 8-5300 eV, 8-1250 eV and 7.8-2100 eV [8], [9], [10]. These measurements extend the previous limited data obtained by Freund et al [11] based on a fast crossed beam technique and avoid some ambiguities arising from the presence of metastable atoms in the fast target beams.

In the case of Mg, cross sections $\sigma_2$ exhibit Auger structure and are found to closely approach our values of $\sigma_1$ at the highest impact energies. In Fe structure in the measured cross sections provides evidence of contributions from inner shell electrons. This structure is less evident in the case of Cu.

## References

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# Theoretical studies on collisions between metallic ions and neutral H, $H_2$, and He

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*(Progress Report for 1st IAEA Research Coordination Meeting on "Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas" September 22-24, 1993, Vienna)*

## 1. Introduction: Theoretical Developments

This work constitutes a considerable extension of an earlier endeavour [1] to assess transfer cross sections for collisions between specific medium-Z metallic ions and neutral H, $H_2$, and He targets. The theoretical method in these investigations is the semiclassical close-coupling method for describing low- and intermediate-energy atomic collisions. This method is appropriate when one deals with sufficiently strong transitions such that perturbation theories break down. It involves the computation of coupling matrix elements between the large number of interacting channels, for the sake of computing transition probabilities to individual final states. This method therefore involves large-scale computations. It may still be considered economic though if there is interest in the *partial cross sections* for populating the many individual final channels.

The semiclassical close-coupling method is known to predict *transfer* cross sections to the *dominant* final $n$-shell of the projectile very well, including its $\ell$-distribution. Predictions on the population of the weaker channels are generally also reliable although not always to all details.

Within the time span of this Coordinated Research Project there has been a growing realization [2] that the description of the weak low-energy *excitation* processes in the target is very difficult, increasingly so with increasing projectile charge. At this point, the best existing calculations [2] for $Z^{Z+}$–H collisions ($Z \leq 6$) at low energies predict strong deviations from the charge scaling of excitation cross sections, that holds at the higher energies. These calculations also predict undulations of the excitation cross sections. Until there is independent confirmation of the predictions of this theory, it has been decided not to engage in extensive calculations on target excitation for further collision systems.

Another development within the scope of this CRP has been the formulation of an efficient description of the one-electron transfer process from $H_2$ *molecules* [3]. This description visualizes the $H_2$ molecule as two adjacent hydrogen-like atoms. The electrons from the two atoms are given the correct binding energy of one electron in $H_2$ by adapting the Coulombic charge of the atoms. The interaction of each of the electrons with all other particles is then approximated by just the interaction between this electron, its associated target quasi-atom, and the projectile. Notably, the electron-electron interaction is hence included only implicitly. On the other hand, the coupled equations are solved *simultaneously* for the process of electron transfer from both target centers. By this formulation we achieve the efficiency of a single-electron description of atomic collisions, and still both electrons contribute to single-electron capture from $H_2$. The formulation guarantees that not more than one two electron can be captured in any collision event. This is an important asset when single-capture probabilities from an hydrogen atom are close to one. Two-electron transfer is however not included.

This model description has been tested for collisions between $H^+$, $He^{2+}$ and $C^{4+}$ projectiles and $H_2$ [3,4]. We find in all cases good agreement with data even for the weak channel.

## 2. New Calculations

Previously, we have studied [1] the $Ti^{4+}$, $Cr^{6+}$, $Fe^{8+}$ – H collision systems at energies of roughly 1 – 100 keV/u. These ions all have the closed-shell electronic core of a $3p^6$ configuration. One hence may assume that the core stays inert in the collisions so that the electron transfer problem is reduced to the problem of one electron moving between the potentials of a proton and a suitably screened charge.

These are the new systems that are being studied now:

- $Ni^{10+}$ –H. This is another example of a system with a closed-shell $3p^6$ core in the projectile. The total transfer cross sections are very close to other systems with equal projectile charge like $Ne^{10+}$ – H. A difference shows up in the $n$-shell distribution of transfer. The slightly larger binding energies of states in the Ni core potential is reflected in a slight shift of the $n$-distribution towards larger $n$ values.

- $Ti^{4+}$ – $H_2$. Calculated total transfer cross sections are close to data for $Ar^{4+}$ and $Fe^{4+}$ projectiles at, respectively, the low- and the high-energy end of our investigation. In the broad energy regime of the maximum of transfer cross section, there is little difference to the calculated cross sections for collisions with atomic hydrogen H. This is well known for other systems and reflects the fact that already the single electron in atomic hydrogen has almost unity probability to transfer to the projectile, in some range of impact parameters, see [4] and references therein. At high energies, the cross sections for the $H_2$ target become larger than the one for the H target as expected. The main contribution to electron transfer comes clearly from the projectile $n$=4 shell (for $Be^{4+}$ it is the $n$=3 shell.

- $Fe^{8+}$ – $H_2$. Similar observations apply, see the previously discussed system.
- $Ti^{4+}$ – He. This system has been studied with a version of the close-coupling description that considers the motion of *two* electrons explicitly, including the electron-electron interaction. Electron transfer populates predominantly the *3d* shell of the projectile (it is the n=2 shell for $C^{4+}$ projectiles). The maximum of transfer cross sections is broader than what has been determined [5] for the $B^{4+}$ – He system. Accordingly, the cross sections at low energies are larger for the Ti system than both experimentally and theoretically for the B system. Two-electron transfer in this system is estimated to be weak, in contrast to the B system [5].

Examples of results are given in the oral presentation to the Research Coordination Meeting, see also the set of copies of the transparencies.

## 3. Outlook

The studies for the systems mentioned in this report are close to completion. Further systems may be investigated in the remaining period of this CRP. This is most worthwhile for systems which cannot easily assessed by applying scaling rules, e.g. systems with low charge states. The final decision will be based on the discussions during the Meeting.

## References

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# IAEA Coordinated Research Program on Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas

## Plasma Impurity Cross Section Data Involving e-Ion, Ion-Atom, Ion-Surface, and Ion-Ion Collisions at ORNL

Progress report by **Charles C. Havener**
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The experimental program at Oak Ridge is centered around a 10 GHz Caprice ECR multicharged ion source. This source has been in operation since Oct 22, 1992, and has replaced the previous ECR source built at ORNL in 1983. Future upgrades of the current source include installation of a metallic oven and development of a direct axial metal feed which will enable the source to provide a wide range of intense metallic ion beams. The ECR source, which has an accelerating potential of up to 25 kV, is used exclusively for atomic physics collision experiments. Our facility maintains a strong collaboration with the group of G. Dunn from the Joint Institute for Laboratory Astrophysics (JILA) at Boulder, Colorado to measure electron collision interactions with multicharged ions. Present on-line experiments in the facility permit the study of electron impact ionization, electron excitation, low energy ion-atom collisions, ion-surface interactions, and ion-ion collisions. A brief summary of our recent activities relevant to this program (data on the medium Z impurities Al, Si, Ti, V, Cr, Fe, Ni, Cu and Ga, high Z impurities Mo, Ta, and W and Kr) is given below.

### 1. Electron impact cross sections for single ionization of multicharged ions.

An electron crossed beams apparatus is used to measure absolute cross sections for electron impact ionization of multicharged ions. The recently modified apparatus can perform measurements at electron collision energies in the range from 30 to 2000 eV with an energy resolution as low as 0.5 eV. This apparatus will be used extensively when the metallic capability of the ECR source becomes operational. Previous measurements with the ORNL PIG ion source which are of interest to this report are summarized in an ORNL Report [1] and more recent measurements (1985-1992, published and unpublished) performed with the current and previous ECR ion sources can also be found in an ORNL Report by D. C. Gregory and M. Bannister, presently in preparation. In all, an extensive list of some eighty target ions, ranging from Z=5 (boron) to Z=92 (uranium) in charge states from +1 to +16 have been investigated at ORNL with this crossed-beam apparatus. Data for several of the ions of interest to this report are included in the 1990 IAEA report [2], more recent data or data not included in that report for Si and Kr ions are: single ionization of $Si^{+}$ and $Si^{2+}$ by Djuric et al.[3]; $Al^{2+}$ and $Si^{3+}$ by Crandall et al. [4], $Si^{4,5+}$ Thompson et al.[in preparation], $Si^{6,7+}$ by P. A. Zeijlmans van Emmichoven et al. [5], and $Kr^{4,5,7+}$ by M. E. Bannister, T. Kojima, and X. Q. Guo [in preparation]. Except where unknown metastable fractions contribute significantly to the measured signal ( e.g., $Si^{2+}$), configuration averaged distorted wave calculations were generally successful in reproducing the observed cross sections for single ionization from both direct and indirect (excitation autoionization) processes.

## 2. Electron impact excitation cross sections.

An electron-merged beams apparatus has been developed by JILA in collaboration with ORNL to measure absolute cross sections for electron impact excitation of multicharged ions. The advantages of this technique include both good energy resolution and complete collection of all electrons. The excitation process which can be studied is not limited to dipole-allowed transitions. One disadvantage is that the collision energy is limited to within a few eV of the threshold region. Of interest to this report are the measurements of the 3s-3p excitation of $Si^{3+}$ [6], and the observed resonant structure in near-threshold excitation of the $4s^2\ {}^1S$ - $4s4p\ {}^3P$ intercombination transition in $Kr^{6+}$ by Bannister et al. (in preparation). Good agreement is found with close-coupling calculations for these and other collision systems ($Ar^{7+}$ and $O^{5+}$) when the observed significant electron backscattering [7] in the near-threshold region is taken into account. When the metallic beams from the ECR source become available, excitation measurements with metallic ions, e.g., Ti, Fe, Cr, and W will be considered.

## 3. Low-energy electron capture cross sections for collisions with multicharged ions and H in ground and excited states.

An ion-atom merged-beams apparatus is used to measure absolute cross sections for total electron capture for collisions with multicharged ions and H in ground and excited states in the energy range between 0.1 - 5000 eV/amu. Advantages of this technique are that the measurements are absolute, there is a large angular collection in the center-of-mass frame, and that the apparatus is able to access the entire range of collision energies. Preliminary $Si^{4+}$ measurements by Havener et al. (unpublished) show a large discrepancy with theory[8,9] below 100 eV/amu. The possibility of insufficient angular collection in the earlier measurements will be addressed by future measurements with the current apparatus which has significantly improved angular collection. Measurements[10] of electron capture (electron loss) from excited H in collisions with multicharged ions fail to show the large n scalings ($n^5$-$n^7$) recently predicted[11] for electron capture at low energies. Recent analysis of the experimental measurements shows that the cross section scales as expected from classical considerations (i.e., $n^4$) even for collision energies below 20 eV/amu where classical CTMC calculations are no longer valid for the range of excited states considered. The ion-atom merged-beams apparatus will be used in conjunction with the future metallic beam capability of the ECR source to provide total electron capture cross sections for a number of ions identified in this report at the very low collision energies where experimental measurements are lacking and scalings do not apply.

## 4. Ion-surface interactions

The neutralization and relaxation process of multicharged ions interacting with a metal surface are also studied in our facility. A highly collimated multicharged ion beam (at keV energies) is incident at various angles (0.2 to 90°) on single crystals of Au, Cu, and Be. The total number and the energy and angular distributions of the emitted electrons are measured. Most of the current investigations have focused on the KLL Auger electron emission observed when incident ions contain inner shell vacancies. This study has led to a relatively good understanding of the neutralization mechanisms in multicharged ion-surface interactions[12]. Recently our understanding of the low energy electron emission due to both kinetic and potential emission processes has increased[13,14] even for velocities significantly above the kinetic threshold. A complication in detailed studies of these low energy electrons is the rapid change of low energy emission from clean metal surfaces as a function of time after sputter cleaning[13]. Certainly, in response to ITER design needs, electron emission during ion bombardment as a function of surface cleanliness can be performed at our facility. Metal surfaces can be studied using the wide variety of ions which can be extracted from the ECR ion source. Future capabilities will include the ability to measure the charge and scattering angle of reflected ions after undergoing interactions with the metal surface.

## 5. Symmetric charge transfer in ion-ion collisions

A single-sourced merged-beam apparatus is under development that will be used to measure relative cross sections for various multicharged ion - multicharged ion symmetric charge transfer collisions, e.g.,

$$Ar^{5+} + Ar^{6+} \rightarrow Ar^{6+} + Ar^{5+}$$

in the energy range between 450 and 1000 eV. This novel self-merged beam technique uses the unanalyzed beam from the ECR ion source and accelerates the beam (with all charge states) into a negatively biased charge exchange cell. Collision products due to symmetric charge exchange in the biased cell are labelled with different E/q when decelerated back to ground potential. A parallel plate analyzer is used to separate the collision products from the primary beams. Theory (which has yet to be tested) for symmetric [15] and quasi-resonant[16] collision systems predict relatively large cross sections ($10^{-15}$ cm$^2$) for these type of collisions.

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Work supported by the Division of Applied Plasma Physics, Office of Fusion Energy, and by the Division of Chemical Sciences, Office of Basic Energy Sciences of the U.S. Dept. of Energy under contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

# ELECTRON IMPACT IONIZATION OF IONS

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## Present status

Two separate crossed beams experimental set-up are presently fully operationnal. The first one is dedicated to the electron impact ionisation studies involving singly charged ions, positive or negative, simple or molecular ions. The second one has been designed for mulptiply-charged ion investigations. It is equipped with an ECR ion source that produces ions essentially from gases. Improvement will be made for an efficient metallic ion production. The electron gun energy range extends from 20 eV up to 6 keV. During the last two years, experiments have been concentrated essentially on rare gas ions, having in mind the completion of data for medium charged states. Single (SI) and double ionization (DI) have been recently analysed for neon, argon and have only started for krypton. The following table indicates charge states for which new data have been obtained. For most of these systems, no crossed beam data were existing up to now.

| | Single ionization | Double ionization |
|---|---|---|
| Neon | q= 6, 8 | q= 5, 6 |
| Argon | 8, 10 | 7, 8, 9, 10 |
| Krypton | tests: q= 8-18 | 7, 8 |

For SI, data are in satisfactoring agreement with theoretical results when these are existing. It is worth mentionning that for some particular cases ($Ar^{9+}$ and $Ar^{10+}$ for instance) semiempirical formula only are available for cross section prediction. For $Ne^{6+}$, excitation-autoionization has been identified from the K-shell to the configuration $1s,2s^2,2p$. This process is of low importance. For $Ne^{8+}$ and $Ar^{8+}$, no contribution from metastable states has been observed.

For DI, the situation is more complex, according to the lack of theoretical predictions. From the experimental results, it is clearly seen that for the highest charge states, DI is dominated by K-shell ionization. For other cases, the position of the first observed ionisation threshold allows the determination of the corresponding ejected electron pair.

For Krypton, data have been published for a charge states not higher then 8, only. Tests have been made on the actual experimental set-up for SI of charge states 8 and 18 and measurement have been performed for DI of $Kr^{7+}$ and of $Kr^{8+}$.

## Future work

As mentionned above, very few data have been obtained for Krypton ions. For this reason, experiments will be performed for this species, for charge states between 8 and 18, the highest one belonging to the argon-like isoelectronic sequence. Both SI and DI will be systematically studied. It is worth mentionning here that the information concerning ionization potentials is not complete for these systems. In particular, inner-shell binding energies (fundamental for DI interpretation) as well as associated excitation ionisation thresholds are not well known. Metallic ions analysis will follow.

## Publications

M. Duponchelle, 1993, thesis, U.C.L.: Electron Impact ionization of multiply-charged neon ions.

Zhang Hui, 1993, thesis, U.C.L.: Electron Impact ionization of multiply-charged argon ions.

Zhang Hui, M. Duponchelle, C. Belenger, E.M. Oualim and P. Defrance, 1993, XVIII ICPEAC, Aarhus, Book of abstracts, p. 369

**IAEA Coordinated Research Programme on**
**Atomic Data for Medium and High-Z Impurities in Fusion Plasmas**

**IAEA Research Agreement No. 6636/CF**
**"Recombination Processes in Electron-Ion Collisions"**

Progress report by

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Recombination in electron-ion collisions can be regarded as one part of a multi-step collision process where in a first step a free electron is captured into a bound state (which can be multiply excited) and in a subsequent decay process photons and/or electrons can be ejected[1]. The final charge state of the ion is determined by the number of electrons ejected from the intermediate electron-ion compound. Thus, a primary ion $A^{q+}$ can finally end up as $A^{(q-1)+}$, $A^{q+}$, $A^{(q+1)+}$, $A^{(q+2)+}$,...

A considerable body of cross section measurements has been reported for the ionization channel subsequent to an initial formation of $A^{(q-1)+}$, i.e. the net production of (singly and multiply) ionized ions after (resonant) electron-ion recombination[2,3]. In the search for such resonant and other contributions to ionization of highly charged ions we have carried out experiments at the Heidelberg storage ring TSR with $Cl^{14+}$ (lithium-like) and $Fe^{15+}$ (sodium-like) ions. Cross sections for single ionization with very good energy resolution and statistics have been measured and fine details could be observed[4]. Detailed comparisons with theoretical calculations of direct ionization, excitation-autoionization, and resonant-excitation-double-autoionization (REDA) are presently being made.

Beside the channel of net ionization also the completed recombination was studied. The center-of-mass energy range covers about $2500eV$ in the case of $Cl^{14+}$ ions and about $1000eV$ in the case of $Fe^{15+}$ ions. Several groups of resonances due to dielectronic recombination were observed and cross sections have been measured. The energy range for $Cl^{14+}$ covers both L-shell and K-shell excitations in the ion core, while for $Fe^{15+}$ ions core excitations from the L-shell and the M-shell were observed[4].

Dielectronic recombination (DR) of $Ar^{15+}(1s^2 2s)$ ions was also studied in a single-pass merged–beams experiment at the UNILAC accelerator of GSI. Absolute recombination rates and cross sections were measured [5] for electron-ion center-of-mass energies from 0 to 580 $eV$.

In the investigated energy range DR produces two groups of resonances. The processes are

$$e + Ar^{15+}(1s^2 2s) \rightarrow \begin{cases} Ar^{14+}(1s^2 2p_{1/2} n\ell) & (n = 10, 11, ..., \infty) \\ Ar^{14+}(1s^2 2p_{3/2} n\ell) & (n = 10, 11, ..., \infty) \\ Ar^{14+}(1s^2 3\ell n\ell) & (n = 3, ..., \infty) \end{cases} \tag{1}$$

Even individual terms in the $1s^2 3\ell 3\ell'$ configuration could be resolved. Theoretical calculations of DR cross sections are in good overall agreement with the data. In the calculations for $\Delta n = 0$ transitions effects of electric fields have to be included to reproduce the magnitude of the measured DR rates at the limit of the $2p_{1/2}n\ell$ and $2p_{3/2}n\ell$ Rydberg series. Discrepancies between theory and experiment are observed at the series limits of the $(1s^2 3\ell n\ell')$ Rydberg series.

The data obtained in similar measurements carried out at the Heidelberg test storage ring TSR for $Li$-like $Cu^{26+}$ ions [6] are less conclusive near the series limits of the $\Delta n = 1$ resonances than the $Ar^{15+}$ measurements, but at lower energies they are of excellent quality and provide very detailed comparisons with theoretical calculations.

Also at the UNILAC, previous experiments with $U^{28+}$ ions were repeated and the energy range was extended to about 500 $eV$. The previous observation[7] of an anomalously high recombination rate at 0 $eV$ center-of-mass energy (i.e. the condition for ion-beam cooling by electrons in a storage ring) was confirmed. A rate enhancement was also observed for $Ar^{15+}$[8] indicating that care has to be exercised with the interpretation of measured radiative recombination rates at very low energies. In a comprehensive research program at the German heavy ion storage rings and at the UNILAC this problem is being investigated and laser techniques are employed to analyze the electron energy distribution in a cooling situation and its impact on electron-ion recombination. The extended measurements with $U^{28+}$ resulted in very rich spectra of dielectronic recombination resonances which are presently being analyzed.

The experimental storage ring ESR in Darmstadt has been employed to study dielectronic and radiative recombination of very high-Z ions such as $Au^{76+}$[9] and $U^{89+}$[10]. For such ions relativistic effects have to be considered both with respect to level energies and transition rates from the highly excited intermediate states populated during dielectronic recombination.

All the experimental facilities will be used for further studies of ionization and recombination of highly charged ions. In some instances data will become available which are directly relevant for fusion (such as $Fe^{15+}$). But also the thorough investigation of other species in collaboration with theoreticians will provide new insight into the physics underlying the data needed for the fusion program and will thus help to improve theoretical predictions of such data.

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# DIRECT ELECTRON-IMPACT IONIZATION OF HIGH-Z IONS FROM THE GROUND AND EXCITED STATES

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## 1. INTRODUCTION

On the basis of the Coulomb-Born approximation with exchange (CBE) calculations for direct ionization [1,2], the fitting parameters were obtained for the cross sections $\sigma$ and Maxwellian rate coefficients $\langle v\sigma \rangle$ for the target states nl: nl = 1s - 6h and for l-averaged values $\sigma$ and $\langle v\sigma \rangle$. These fitting parameters are required for solving plasma kinetic problems: line intensities, impurity transport, radiative losses, etc.

## 2. RESULTS

Fitting parameters obtained are smooth functions of quantum numbers n and l. For high n-states the l-averaged ionization cross sections are in good agreement with classical impulse approximation, which was also considered in this work. The accuracy of cross sections and rate coefficients, obtained with the help of fitting parameters is within 15% as compared to numerical CBE calculations.

The calculations of $\sigma$ and $\langle v\sigma \rangle$ are presented for ions $C^{2+}$, $Ne^{3+}$, $O^{4+}$ $Si^{6+}$, $Si^{7+}$, $Ni^{14+}$, $Cr^{10+}$ in comparison with experiment and recommended data.

## 3. CONCLUSIONS

Fitting parameters of cross sections and rate coefficients for direct ionization of ions $X_z(nl)$ by electron impact from the states $1s \leqslant nl \leqslant 6h$ as well as for $nl = ns, np, nd$ $(n \geqslant 7)$ and l-averaged values $(n \geqslant 7)$ were evaluated on the base of direct ionization cross sections (and rates) of multicharged ions from the ground and excited states, including ionization of inner-shell target electrons.

The range of the incident electron energy E (and temperature T) considered is limited by relation $E < 15I$ $(0.1I < T < 8I)$, where I is the binding energy of the target electron shell. This energy and temperature range is usually the most interesting for practical physical applications.

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# EXPERIMENTAL AND THEORETICAL CROSS SECTION DATA FOR SINGLE ELECTRON CAPTURE IN COLLISIONS OF Si, Ti, Ni, Mo and W IONS WITH H, $H_2$ and He.

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## ABSTRACT

A compilation and evaluation have been made of existing experimental and theoretical cross section data for total electron capture of Si, Ni, Ti, Mo and W highly charged ions with H, $H_2$ and He.

## INTRODUCTION

One of the reactions of relevance to a better understanding of the plasma edge and neutral beam diagnostics is electron capture. Atomic and molecular data for metalic impurities in fusion plasmas are still inadecuate to meet the needs in the current energy research programme.

We have compile the experimental and theoretical cross sections for single electron capture processes

$$A^{q+} + B \dashrightarrow A^{(q-1)+} + B \quad (1 \le q \le Z) \qquad 1)$$

where A = Si, Ti, Ni, Mo and W and B = H, $H_2$ and He.

In most of the cases no coincidence analysis with respect to the charge states of the target ions after the collisions has been performed. Therefore, the experimental data may contain also contributions from the transfer ionization process; other process such as for $H_2$ targets, dissociative collision channels which may involve charge transfer and ionization or two electron process with capture and ionization for the case of He must be considered, however no detail information has been found in the literature.

The cross sections data for the reaction 1) are found in several publications and the comments which appear in Refs. 1) and 2) with regard for the same reaction but for other ions are also valid for the ions discussed here.

The availability of the data for collisions $A^{q+}$ + B are presented in the table and corresponds to all the data in the literature as of December 1992 regardless any degree of reliability. Since previous compilation, Refs. 47 - 54 only few investigations have been reported. The results of a critical analysis according to evaluation procedures, based on established criteria are presented in a special volume with the corresponding Chebychev polynomial fit to the data.

It can be noticed from the table I that both experimental results and theoretical calculations are needed for this systems. For instance, charge transfer collisions between He and Ti, Ni, Mo and W ions need to be investigated both experimentally and theoretically, since He constitute the ash of ignited D - T plasmas and it will be abundant in the edge plasma.

An effort is been made to measure at least low energy, low charge exchange cross sections for some of the systems already mention. The need for such data has been full documented in Refs. 56 - 58.

## TABLE 1

### Total Electron Capture Cross Section Data for $Si^{q+}$, $Ti^{q+}$, $Ni^{q+}$, $Mo^{q+}$ and $W^{q+}$ with H, $H_2$ and He.

| Ion/Target | H | $H_2$ | He | References |
|---|---|---|---|---|
| $Si^{2+}$ | T X | X | | 3-9, 10, 11-24, 33-36, 38, 43, 45-49, 50, 52, 53, 55 |
| $Si^{4+}$ | T X | X | T | |
| $Si^{5+}$ | T X | X | | |
| $Si^{6+}$ | T X | X | | |
| $Si^{7+}$ | T X | X | | |
| $Si^{8+}$ | T + | X | X | |
| $Si^{9+}$ | T + | + | | |
| $Si^{10+}$ | T | | | |
| $Si^{11+}$ | T | | T | |
| $Si^{12+}$ | T | | | |
| $Si^{13+}$ | T | | + | |
| $Si^{14+}$ | T | T | T | |
| $Ti^{2+}$ | X | | | 10, 16, 22, 24, 27-34, 36, 40-42, 47-49, 50 |
| $Ti^{4+}$-$Ti^{22+}$ | T | | | |
| $Ni^{4+}$-$Ni^{28+}$ | T | | | 10,16,24,33-36,41,42, 45,47,48,50,53 |
| $Mo^{4+}$ | T + | + | | 7, 10, 16, 22, 33-35, 50 |
| $Mo^{5+}$ | T + | + | | |
| $Mo^{6+}$-$Mo^{17+}$ | T X | X | | |
| $Mo^{18+}$ | T X | | | |
| $Mo^{19+}$-$Mo^{30+}$ | T | | | |
| $Mo^{42+}$ | T | | | |
| $W^{4+}$ | T + | + | | 7, 10, 16, 22, 24, 34, 35, 37, 47, 49, 50 |
| $W^{5+}$ | T X | X | | |
| $W^{6+}$ | T X | X | | |
| $W^{7+}$ | T X | | | |
| $W^{8+}$ | T | X | | |
| $W^{9+}$ | T X | X | | |
| $W^{10+}$ | T X | X | | |
| $W^{11+}$ | T X | X | | |
| $W^{12+}$ | T X | X | | |
| $W^{13+}$ | T | | | |
| $W^{14+}$ | T + | + | | |
| $W^{15+}$ | T + | + | | |
| $W^{16+}$-$W^{30+}$ | T | | | |
| $W^{74+}$ | T | | | |

X: Experiment; T: Theory; +: only one experimental datum

Acknowledgments. This work has been partially supported by DGAPA, grant IN104391, CONACYT and IAEA, Research Contract No. 6720/R1/RB.

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IAEA Coordinated Research Programme on Atomic Data for Medium and High Z Impurities in Fusion Plasmas.

Research Agreement No. 6635/CF

# "CTMC Study of Medium- and High-Z Ions Collisions with H, $H^*$, He and $He^+$"

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Work in progress in the unit of Atomic Physics of Fusion Plasmas (PAPF) of the Laboratory of Gases and Plasma Physics (LPGP) at Orsay is partly related with the evaluation of ion - atom collision cross sections of interest to fusion, total for ionization and total and partial (n,l resolved) for charge transfer. In collaboration with the group of theory of the LPGP and with external collaborations we have calculated "ab initio" an extensive amount of cross sections. This work resulted to sets of evaluated data which have been stored in form of parametrized curves in order to be handy for everyday use, but also for being directly used in modelling of fusion plasmas. Both Chebyshev polynomials and empirical formulas have been used for these parametrizations [1,2].

Data have been evaluated for the following processes:

$A^{q+}$ + H collisions
Energy range: 10 ev/amu to 5 Mev/amu
One $e^-$ ionization cross sections.
One $e^-$ charge transfer,
total cross sections all $Z < 75$, all q;
partial n-resolved cross sections, q=3 to 8.

$A^{q+}$ + He collisions, totally stripped ions, Z = 1 to 28
Energy range: 1 kev/amu to 1 Mev/amu
Simple and double ionization cross sections.
Simple and double total charge transfer.

$A^{q+}$ + $He^+$ collisions, totally stripped ions, Z = 1 to 18
Energy range: 1 kev/amu to 5 Mev/amu
Ionization and total charge transfer cross sections.

The programme involved the following theoretical studies based in the CTMC approximation:

1. Study of charge transfer in $A^{q+}$ + H, $H^*$ collisions within the approximation of Coulomb potential interaction.

In continuation of our previous calculations [3,4,5] we have extended the Z values of the $A^{q+}$ projectiles up to Z = 74 ($W^{q+}$). Typical results for Mo and W are presented in Fig. 1. Additional calculations are under way in order to complete the total cross section evaluations for projectiles of any Z between 3 and 74.

2. Calculation of n-resolved partial cross sections for $A^{q+}$ + H collisions for any Z. Although the results obtained using Coulomb potentials are in principle valid for totally stripped ions, a

satisfactory approximation can in general be obtained for highly ionized atoms provided that the remaining shell electrons have not an important correlation with the active electron [6]. Unpublished results concerning $A^{8+}$ + H collisions are shown in Fig. 2.

3. Target ionization in $A^{q+}$ + $H,H^*$ collisions. Calculations in a wide energy spectrum for q = 1 to 74 allowed a comparison with existing results and the definition of the validity range of the well known Gillespie formula (see Fig. 3).

4. Charge transfer (including n-resolved partial cross sections) in collisions of $A^{q+}$ with He atoms. It has been previously shown [7] that the Independent Electron Model (IEM) is inadequate for He targets. Therefore we have developed a sequential approximation (ns-CTMC) in order to properly describe the interaction of the second target electron, also using a non-Coulomb potential. Preliminary data, presented in a recent meeting [8] are shown in Figs. 4 and 5. These results allowed the critical evaluation of formulas previously used for the charge transfer cross sections for $A^{q+}$ + He collisions. Fig. 4 is showing a comparison of our results with these formulas. Fig. 5 gives an example of n-resolved partial cross sections for the case of $Be^{4+}$ + He collisions.

5. Target ionization in $A^{q+}$ + He collisions. Calculations for q = 1 to 18 have been recently achieved. The use of ns-CTMC is giving the correct evaluation of the double ionization of the target. Therefore, the ratio $\sigma^{+}/\sigma^{++}$ of the simple versus the double ionization cross sections becomes higher (see Fig. 6).

6. Charge transfer and target ionization in $A^{q+}$ + $He^{+}$ collisions. A series of calculations for q = 1 to 18 led to conclusions on the electron capture by the $A^{q+}$ projectile, on the ionization of the $He^{+}$ target and on the electron removal from the target (see Figs. 7,8 and 9).

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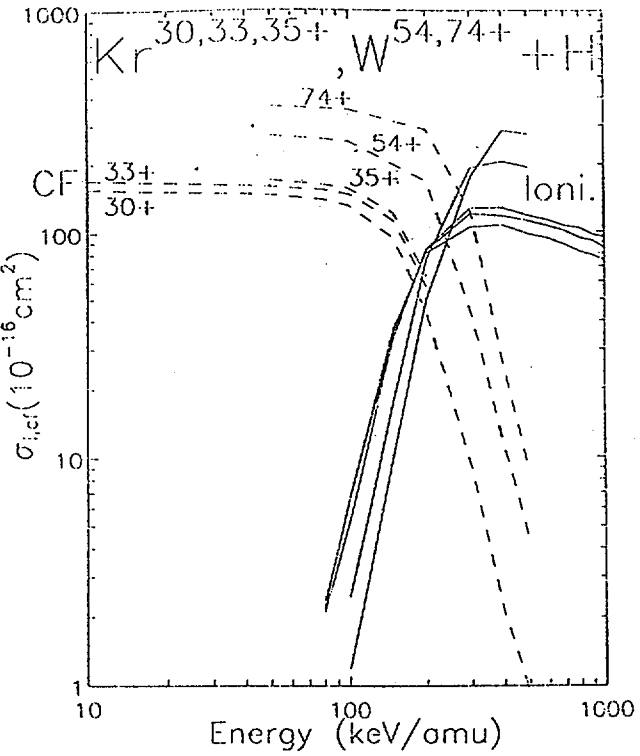

Fig. 1

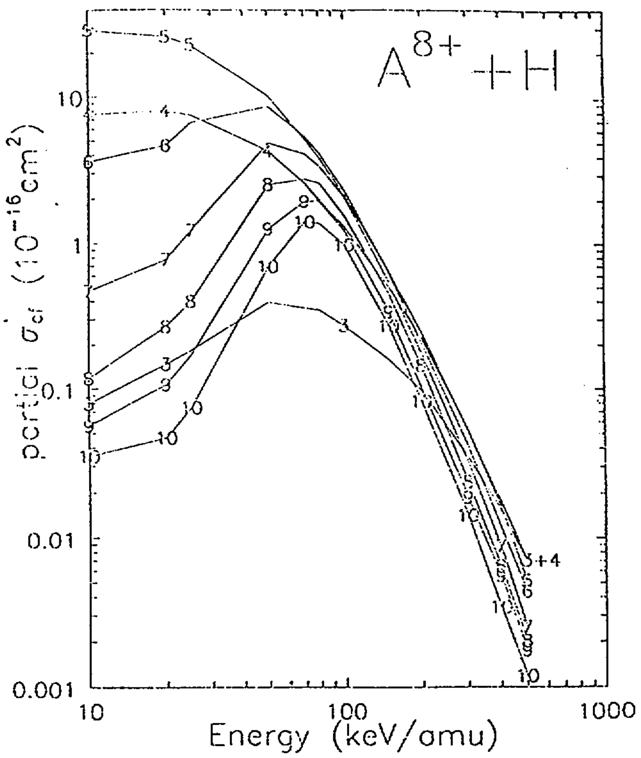

Fig. 2

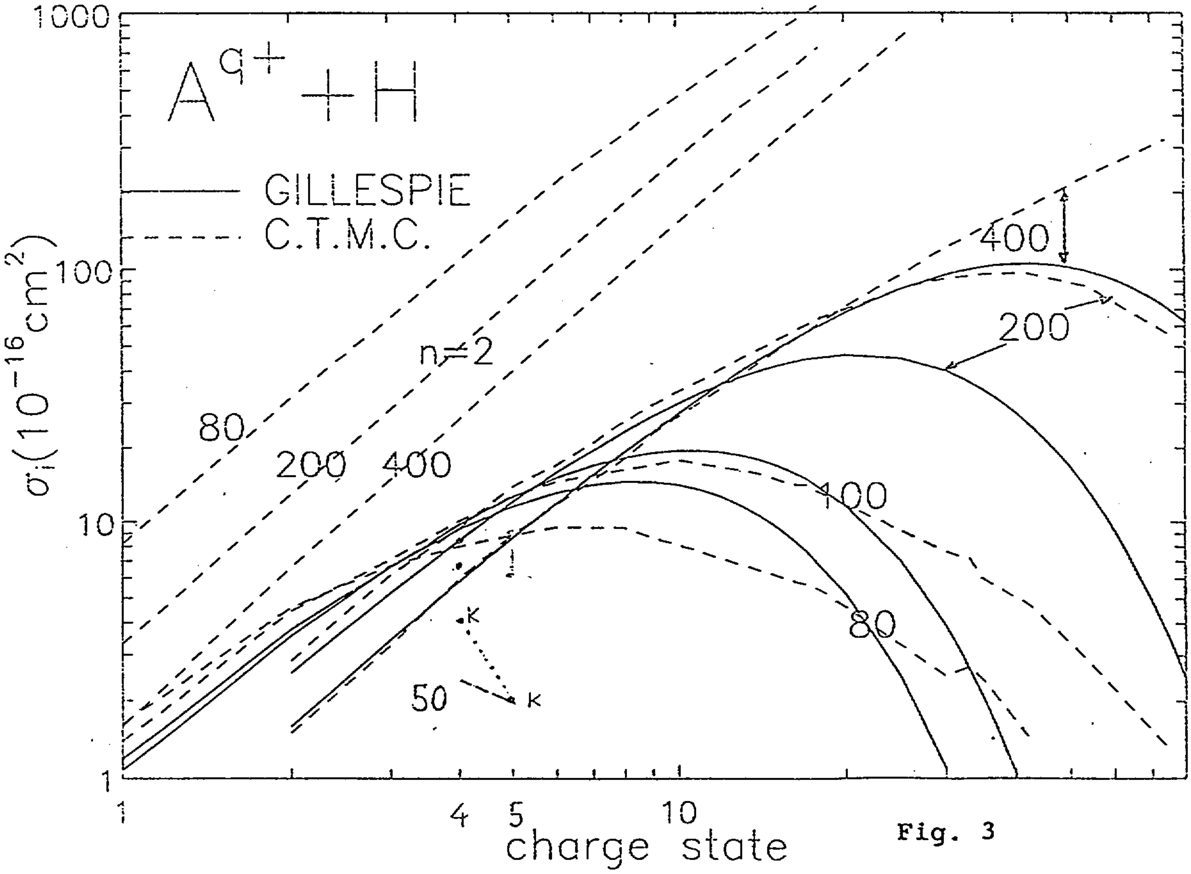

Fig. 3

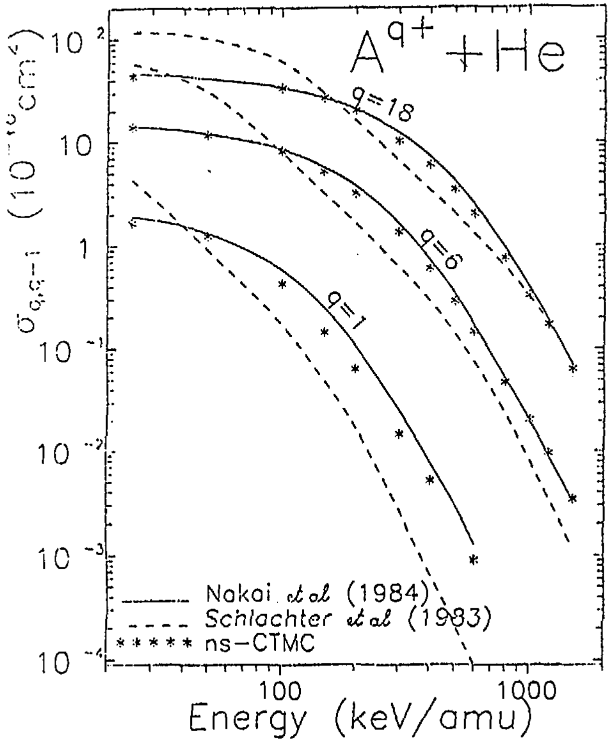

Fig. 4

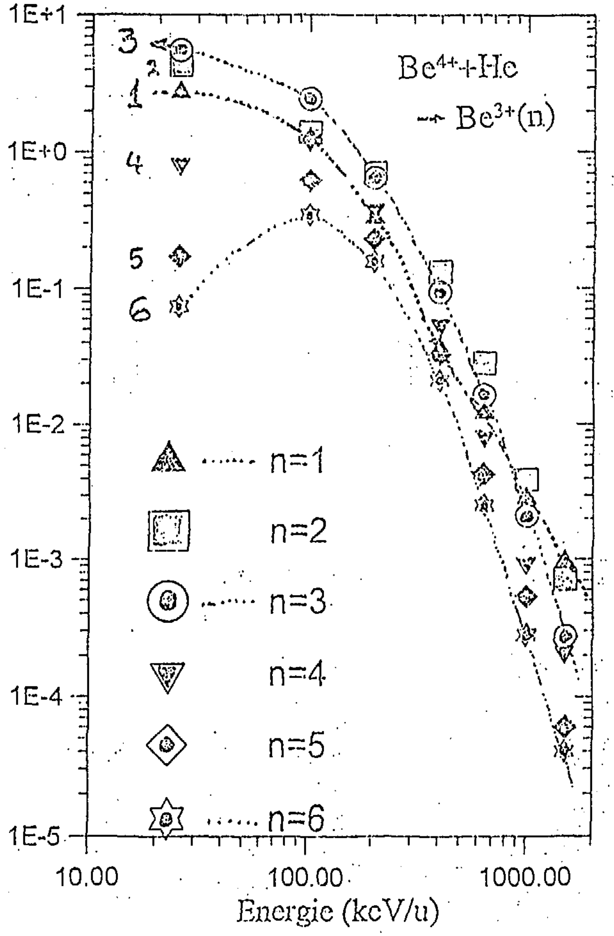

Fig. 5

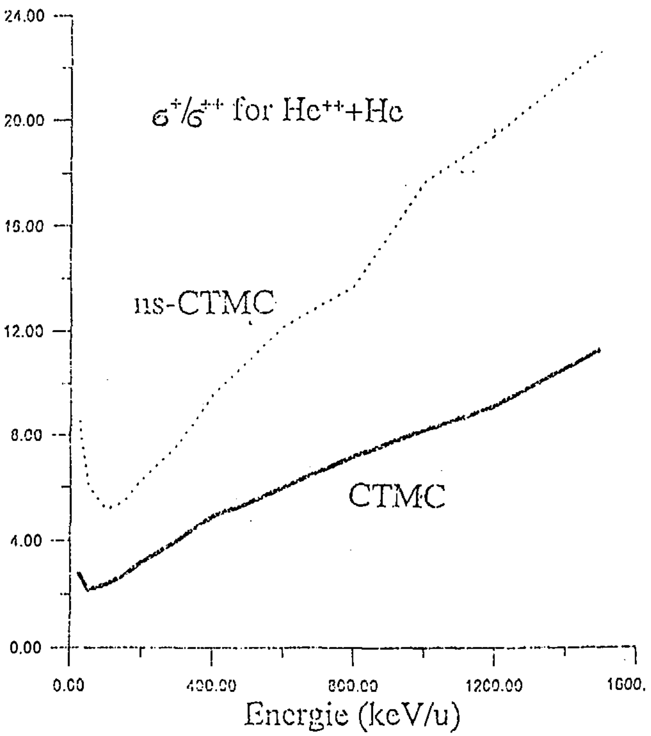

Fig. 6

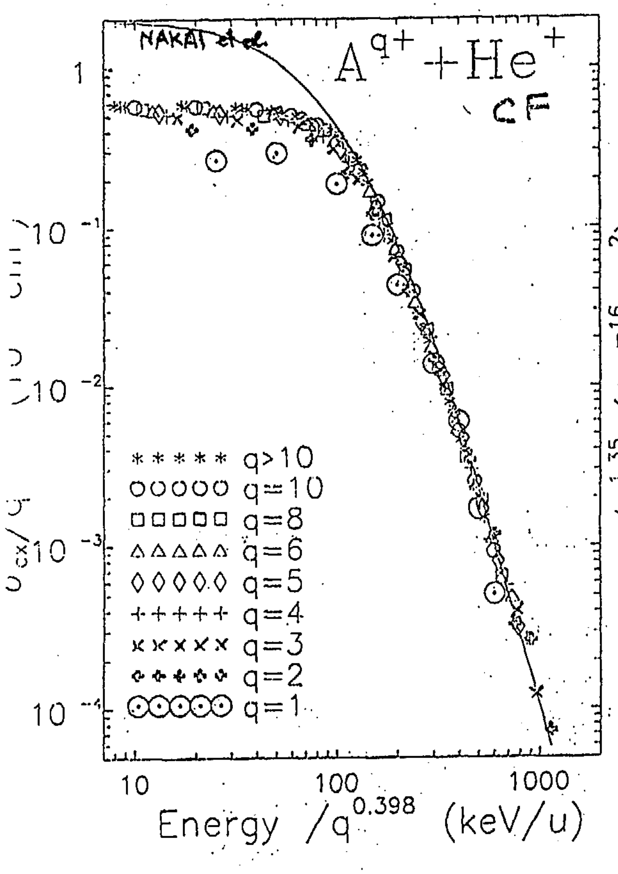

Fig. 7

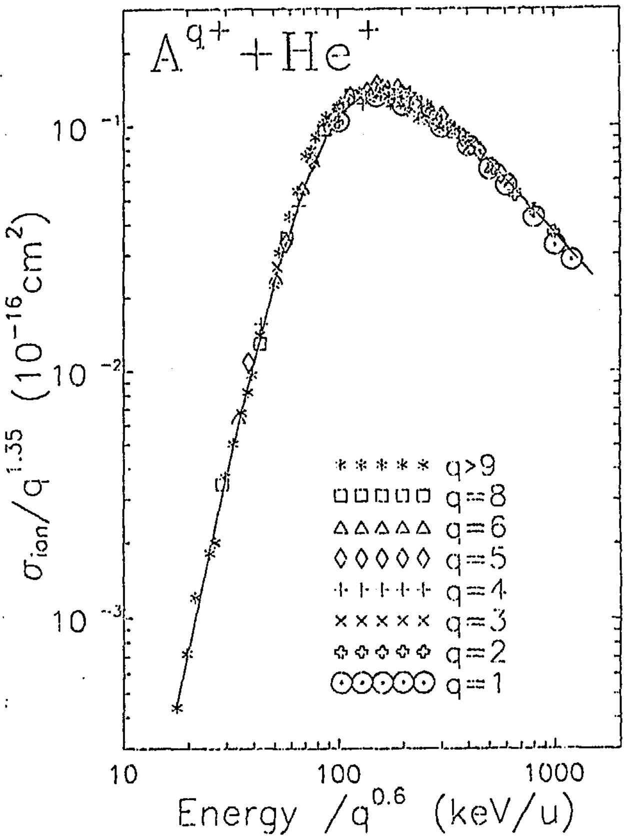

Fig. 8

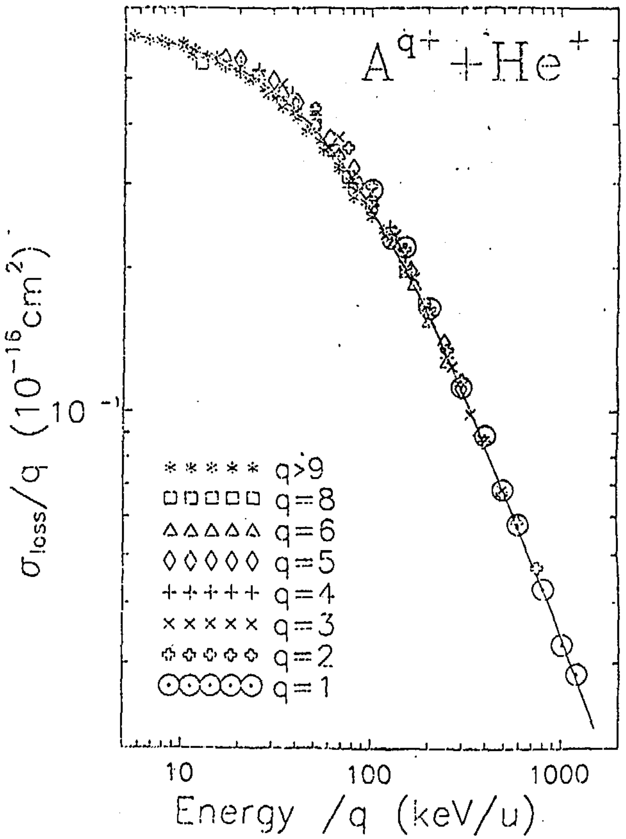

Fig. 9