REPORT NO. IAEA-R-2043-F

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TITLE

Theoretical study of charge exchange, ionization and electron loss processes, relevant to controlled thermonuclear research

FINAL REPORT FOR THE PERIOD

1977-02-01 - 1980-02-28

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IAEA Research Contracts:
No 2043/RB, No 2043/R1/RB
No 2043/R2

FINAL REPORT

I. GENERAL INFORMATION ON THE PROJECT

1. Contract Numbers: 2043/RB; 2043/R1/RB; 2043/R2/RB

2. Title of Project: "Theoretical study of charge exchange, ionization and electron loss processes, relevant to controlled thermonuclear fusion research".

3. Institute where the research was carried out: Institute of Physics, Dept. of Theoretical Physics
Studentski trg 12/V
P.O. Box 57
11001 Beograd
Yugoslavia

4. Chief scientific investigator: Dr Ratko JANEV

5. Time period covered:
July 1, 1977 - February 28, 1981.

II. DESCRIPTION OF RESEARCH CARRIED OUT

2.1. Scope of the problems investigated and their relevance to fusion research

During the period covered by the Research Project, the following groups of physical processes have been investigated:

a/ Electron capture processes in low - and high -energy collisions of multiply charged ions with atoms and molecules /including single - and two - electron capture/.

b/ Excitation and ionization processes in low - and high - - energy collisions of atoms with multiply charged ions.

c/ Ion - ion recombination and ion - pair formation processes in slow collisions involving hydrogen and alkali atom /ion/ partners.

d/ Ion /atom/ - solid surface collision processes.

The studies of inelastic collision processes involving multiply charged ions /items a/ and b/ are directly related to the "impurity problem" in tokamak plasmas /ionization equilibrium, radiation and particle losses, etc./, the efficiency of neutral beam heating method /beam penetration and energy deposition/, plasma diagnostics and modelling.

The processes under items c/ and d/ are related to the neutral beam production /processes in the ion sources/ and transport/ processes in the ion beam neutralizers/, as well as to the plasma - wall interaction problem.

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For most of the considered processes within the above broad classes, original approaches have been developed and, in illustrating the theoretical results, atomic species and collision energies of direct importance for the fusion research have been chosen.

2.2. Description of the processes investigated and the theoretical methods used

1/ Single electron capture in atom - highly charged ion collisions at low energies

The process

$$A + B^{Z+} \rightarrow A^{+} + B^{(Z-1)+} \qquad (1)$$

/A, B are any atoms, Z is the net ionic charge/ has been investigated [1*] using the concept of electron tunnelling through barrier created between the atomic and ionic potential wells during the adiabatic collision. The transition probability per unit time is obtained in analytical form. The general dependences of the cross section on the parameters of the problem /Z, collision velocity V , initial state electron binding energy I_o, etc/ are obtained analytically. Cross section /σ/ calculations for reaction /1/ are performed [1,36] for A = H, H_2, inert gas atom and B^{Z+} = fully /or highly/ stripped ion in the energy region below 100 keV /collision velocity ($v \leq Z^{1/4}$, in atomic units/. The scaling properties of σ/with respect to Z and I_o/ are also investigated [3,6], and the mosly populated final state level in reaction /1/is determined [3].

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* A supperscript hereafter refers to the paper from the list of publications /Section V/.

For the $H + Z \rightarrow H^+ + /Z-1/$ /Z=fully stripped ion/ reaction a classical model has been analytically developed[7] for the low and intermediate collision energies. Cross section calculations were performed[7] for: Z = 8, 1o, 14, 18, 26, 36. Both the tunnelling and classical models give results in good agreement with the availble experimental data and theoretical relusts of more involved numeracial computations.

In the high energy region, the problem of electron capture from the inner electronic shells has been studied[8] within the Born approximation. Suitable paramatrizations tor the partial and total cross sections and the collision energy were established. Calculations for electron capture from the K -, L -, and M - shells of Ar in collisions with multicharged ions were performed for projectiles with $Z \lesssim 50$.

2. Two-electron capture in ion-atom low-energy collisions

Using the Landau-Herring method, the two-electron exchange interaction in the asymmetrical diatomic systems has been calculated asymptotically exactly[9]. The result for the symetrical case is obtained as a special case. On the basis of this result the cross section for the two-electron charge exchange reactions $He^{2+} + He \rightarrow He + He^{2+}$ and $C^{4} + He \rightarrow C^{2+} + He^{2+}$ were calculated[9]. Good agreement with the existing experimental data was obtained. The two-electron capture in atom-multicharged ion slow collisions has also been treated within the tunnelling and classical absorption model [15]. Approximate relations between the single-electron and two-electron capture cross sections have been obtained[15], in satisfactory agreement with the experimental data.

3. Excitation of atoms in collisions with multiply charged ions

The single-electron excitation process of atoms colliding with multiply charged ions has been considered using the atomic-state-based close-coupling method and the dipole

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approximation for the ion-atom interaction [10]. The corresponding close-coupled equations for ns→n'p transitions have been solved approximateby by the Veinshtein-Presnyakov-Sobelman method and the excitation cross section is calculated analytically /expressed in term of an integral/. Scaling relationships for the excitation cross section have been ruled aut [10] in low, intermediate and high energy regions. Cross section calculations have been performed for Z=1-32 /in the energy range from 10-1000 keV/amu.

4. Impact ionization of atoms by multiply charged ions

Introducing the concept of an effective oscillator strength for single electron transitions into the continuum, the impact ionization of atoms by multicharged ions has been considered [10] within the two-and three-state close - coupling method and the dipole approximation for the ion-atom interaction. Expressions for the cross section are obtained in closed form, valid for the low, intermediate and high energy. Cross sections calsulations have been performed for H /1s/ + + $Z \rightarrow H^+ + Z + e$ [10] and He /$1s^2$/ + $Z \rightarrow He^+ + e$ [17] ionization reactions /with Z = 1-32/ in the energy region form 10 keV/amu to several MeV/amu.

A second order quantum theory for the ionization process in the high energy ion-atom collisions has been deveoped [4], based on the continuum intermediate state method. Cross section calculations have been performed for the H /1s/ + p^4 and H /1s/ + He^{2+} [11] ionizing collisions in the energy region above 50 keV, showing a good agreement with the experimental data.

Non-relativistic bound-free transition form factors have been calculated analytically for the hydrogen atom [16].

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5. Ion-ion recombination and ion-pair formation

Cross section and reaction rate coefficients have been calculated in the low energy region /$\lesssim$10 keV/ for the processes $H^- + M^+ \rightarrow H + M$ /*/, where M denotes an alkali metal atom. The multi curve-crossing Landau-Zener theory has been used with improvment which accounts for the correct R-dependence of the coupling matrix elements and the finitness of the nonidabatic transition zones. The cross section for the $Cs + D \rightarrow Cs^+ + D^-$ reaction is compared with the experimental data /E = 0,5 to 10 keV/, showing a satisfactory agreement with the experimental data.

6. Resonant processes in ion /atom/ low energy collisions with partially covered solid surfaces

The processes of resonant ionization of atoms and resonant neutralization of ions slowly colliding / E $\gtrsim$ a few KeVs/ with metal surfaces covered by an atomic sub-monolayer have been considered [12]. The corresponding electron transition probabilities are calculated by using a non-perturbative approach to the problem and representing the surface ad-atoms by finite dipoles. The influence of the surface sub-monolayer on the probability of considered processes is investigated. It is demonstrated [13] that the survival probability of hydrogen negative ions emerging from a Cs-coated tungsten surface, is by factor of about 100 greater than the corresponding probability in the case of a clean surface.

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7. Auger de - excitation of metastable atoms on metal surfaces

A new, nonperturbative approach for the process of Auger de-excitation of metastable atoms, slowly colliding with a metal surface, is developed [19]. The applied method is analogous to the one used in the problem of Penning ionization in atom-excited atom collisions. The developped theory is applied to the de - excitation collisions of He / 2^3S/ and He^+ /n/ with the Mo /loo/ surface.

III. RESULTS OBTAINED

The results obtained within the Research Project are partially mentioned in the preceding Section. The results of the research, are included in 2o publications /15 published and 5 in the course of publication/. Among these, 5 articles/Refs: 5, 14, 15, 18, 2o/ have a review character. We shall now summarize the most important resulsts of our investigations:

a/ Theorectical models /or methods/ have been developed for the charge exchange [1, 6, 7, 9], excitation [1o] and ionization [4, 1o] processes in atom-highly sharged ion collisions at both low and high collision energies. Concrete cross section calculations for reactions of direct relevance to the controlled thermonuclear research have been performed [1,3 - 11, 17], using the developed theories. Some scaling laws have been established for the considered processes.

b/ Ion-ion recombination and ion-pair formation processes in hydrogen-alkali diatomic systems have been treated /cross section and reaction rate calculations/[2].

c/ A theoretical model for the atomic collision resonant processes on a covered surface has been developed [12], and applied in calculations of the survival probability of hydrogen negative ions, emerging from Cs-coated W and Mi surfaces [13].

d/ A theoretical approach for Auger de-excitation of metastable atoms, slowly colliding with solid surfaces, has been developed and applied He / $2\,^3S$/ and He^+ /n/ collisions with Mo /100/ surface [19].

e/ A number of reviev articles has been written on the processes investigated within this Reserch Project [5, 14, 15, 18].

IV CONCLUSIONS

A good piece of work has been done in the frame of the Research Project No 2043/RB. The processes investigated are of great importance for the magnetic fusion research from the point of view of both plasma heating and cooling, and plasma diagnostics and modelling. Of particular importance in this context are the results obtained within the Project which pertain to the collision processes of multiply charged ions with atoms. The established scaling laws for the low energy charge exchange and for the impact excitation and ionization in various energy regions have a great impact to the plasma modelling work energy balance estimates, neutral beam heating, etc.
The efficiency of the "plasma-surface sources" for negative hydrogen ion production is now explained by the high survival probability of n gative hydrogen ions, emerging from Cs-coated surfaces /a factor of 100 with respect to the case of clean surfaces/.

The future theoretical investigations along the line of research covered by the present Project should, in our opinion, include:

a/ Establishing of Z-scaling laws for the charge exchange cross section in the intermediate collision velocity region /$V \sim Z^{1/4}$ a.u./

b/ Investigation of the question whether a given scaling law for the charge exchange or ionization process will remain valid for very large values of Z/still within the non-relativistic region/.

c/ Derivation of analytical expressions for the distribution of captured electrons over the /n, ℓ/ final state quantum numbers.

d/ Precise multistate close-coupling cross section calculations for some particular reactions / of charge exchange or ionization type / needed for plasma diagnostics.

e/ Investigation of collision processes of highly charged ions with solid surfaces.

During the work on the present Project we got a feeling that organization of a coordinated international research programme on a specific group of collision processes relevant to fusion research would be an efficient way to meet the urgent requirements imposed on the atomic physics work by the fusion research.

V. LIST OF PUBLICATIONS

/Papers published on the work done under the contract/

1. T.P. Grozdanov, R.K.Janev
Charge exchange collisions of multiply charged ions with atoms.
Phys.Rev. A17 , 88o /1978/.

2. R.K. Janev, Z.M.Radulović

Ion-ion recombination and ion-pair formation processes in alkali-hydrogen diatomic systems.

Phys. Rev. A 17 , 889 /1978/

3. T.P. Grozdanov, R.K. Janev

One-electron capture in slow collisions of highly charged ions with atoms.
Phys. Lett. 66A , 191 /1978/.

4. Dž S.Belkić

A Quantum theory of ionization in fast collisions between ions and atomic systems.
J. Phys B. 11 , 3529 /1978/.

5. Dž S.Belkić, R.Gayet, A.Salin

Electron capture in high-energy ion-atom collisions
Physics Reports 56 /N 7/ 1979.

6. T.P.Grozdanov, R.K.Janev

Electron capture in slow collisions of multiply charged ions with hydrogen molecules.
J.Phys. B 13 , L69 /198o/.

7. T.P. Grozdanov
Classical model for electron capture in collisions of highly charged, fully stripped ions with hydrogen atoms.
J.Phys. B , 13 3835 /198o/.

8. R.K. Janev, L.P. Presnyakov, V.P.Shevelko

One-electron capture from the inner shells
in atom-multicharged ion collisions.
Phys.Lett. 76A , 121 /1980/.

9. T.P. Grozdanov, R.K.Janev
Two-electron capture in slow ion-atom collisions
J.Phys. B 13 , 3431 /1980/.

10. R.K.Janev, L.P. Presnyakov

Single electron excitation and ionization processes
in atom-multicharged ion collisions.
J.Phys. B 13 , 4233 /1980/

11. Dž.Belkić
Chrage dependence of ionization cross sections
J.Phys B 13 , 1394 /1980/

12. R.K.Janev, S.B.Vojvodić

Interaction of atomic particles with solid surfaces.
IV. One - electron resonant processes in the presence
of a surface sub-monolayer.
J.Phys B 13 , 2481 /1980/.

13. R.K.Janev, S.B. Vojvodić

Survival probabilities of hydrogen negative ions
emerging from Cs-coated W and Ni surface.
Phys.Lett. 75A , 348 /1980/.

14. R.K.Janev
Ionization and electron loss of hydrogen atoms by
highly charged ions.
Physica Scripta 23 , 180 /1981/.

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15. R.K.Janev, L.P. Presnyakov
Collision processes of multiply charged ions with atoms
Physics Reports, /March issue, 1981/

16. Dž. Belkić
Bound-free nonrelativistic transition form factor in atomic hydrogen
J.Phys. B /1981; accepted for publication/

17. R.K.Janev
Impact ionization of helium atoms by multiply charged ions
Phys.Lett. /1981; accepted for publication/

18. R.K.Janev, T.P.Grozdanov
Charge exchange processes in atom-multicharged ion collisions.
Invited lecture given at X SPIG, Dubrovnik 1980
To appear in: "The Physics of Ionized Gases", Ed M.Matić, Beograd, 1981.

19. R.K.Janev, M.N.Nedeljković
Interaction of atomic particles with solid surfaces
V. Auger de-excitation of metastable atoms
J.Phys B /submitted for publication/

20. R.K.Janev, P.Hvelplund
On the cross section scaling laws for charge exchange,ionization and electron loss proceses in atom-highly sharged ion collisions
Comment in At.and Mol.Phys. /1981, to appear/

March 3, 1981
Belgrade

Principal Investigator
Dr Ratko Janev

R. Janev

Eclosures:
1/ Project expenditures
2/ Summary of the Project

SUMMARY

ON THE WORK PERFORMED UNDER THE IAEA RESEARCH PROJECT:
R.C. Nos: 2043/RB; 2043/R1/RB and 2043/R2/RB

1. Title of Project: "Theoretical study of charge echange, ionization and electron loss processes, relevant to controlled thermonuclear fusion research".

2. Research Institute: Institute of Physics
Dept. of Theoretical Physics
Studentski trg 12/V, P.O. Box 57
11001 Beograd /Yugoslavia/

3. Chief Scientific Investigator:

Dr Ratko JANEV

4. Period of Contract: July 1. 1977 - February 28. 1981.

5. Scientific Backgroung and Scope of Project:

The investigation of atomic collision processes has a great impact to the present-day controlled thermonuclear fusion research /energy balance, particle transport, plasma heating and cooling, plasma modelling and diagnostics, neutral beam heating, etc/. Within the Research Project No 2043/RB and its two renewals the following processes have been studied:

a/ Single and double charge exchange in low, medium and high energy collisions of atoms with multiply charged ions;

b/ Excitation and ionization processes in low, medium and high energy collisions between multiply charged ions and atoms;

c/ Ion-ion recombination and ion-pair formation collision processes between hydrogen and alkali atoms /ions/;

d/ Resonant and Auger processes in slow collisions of atomic particles with solid surfaces /including surfaces covered by a sub-monoatomic layer/.

Processes a/ and b/ are important for the "impurity problem" of magnetically confined tokamak plasmas, whereas processes c/ and d/ for the production and transport of intense neutral beams for plasma heating.

6. Methods used in the investigations

For most of the processes investigated, original theoretical methods and approaches have been developed. This includes: an electron tunnelling model for single electron capture in atom-highly sharged ion low energy collisions, a classical model for the same process at intermediate energies, an analytical and three-state close-coupling dipole approximation for the excitation and ionization processes in atom-highly charged ion collisions, a second order non-perturbative method for impact ionization, an asymptotic method for the two electron capture process, a non-pertirbative method for charge transfer atom /ion/-surface collision processes, etc.

7. Results obtained

Appart from the development of above mentioned methods for studying the collision processes which are of interest to the controlled thermonuclear fusion research, probability, cross section and reaction rates data have been produced for a large number of concrete reactions.

The reactants and the energy ranges for which these data are produced have a direct relevance to the magnetic fusion research and may be /and already are/ used in plasma modelling calculations, plasma-wall interaction studies, neutral beam penetration and beam energy deposition, etc. Of special importance for the fusion studies are the cross section scaling laws which have been established for most of the processes investigated.

The results obtained are published in 2o publications, 5 of which are invited review articles or lectures at international scientific meetings.

8. Conslusions

The work performed within the present Project has yealded important information on the collision processes considered, both from pure scientific point of view and from point of view of its practical application in the controlled fusion research. During the research within this Project, the most important next steps of investigation of these processes are identified. It is felt that an international coordination of the research in this field would be very useful for more efficient production of atomic and molecular data, required in the fusion research.

9. Papers Published on Work Done under the Project

1. T.P. Grozdanov, R.K.Janev

Charge exchange collisions of multiply charged ions with atoms.
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5. Dž. S. Belkić, R.Gayet, A.Salin

Electron capture in high-energy ion-atom collisions.
Physics Reports 56 /No6/ 1979.

6. T.P. Grozdanov, R.K. Janev

Electron capture in slow collisions of multiply charged ions with hydrogen molecules.
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Classical model for electron capture in collisions of highly charged, fully stripped ions with hydrogen atoms
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8. R.K. Janev, L.P.Presnyakov, V.P. Shevelko

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11. Dž. Belkić

Charge dependence of ionization cross sections
J.Phys. B 13 , L593 /1980/.

12. R.K. Janev, S.B. Vojvodić

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