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Atomic Processes in High Temperature Plasmas

by

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Abstract

This is the final report on the project 'Atomic Processes in High Temperature Plasmas', which has been completed in June 30, 1991. The original contract started in 1978. The dielectronic recombination (DR) rate coefficients were calculated for ions with the number of electrons $N = 1, 2, 3, 4, 5, 10, 11$, and 12. The result was then used to construct a new and improved rate formula. Other important resonant processes, which are closely related to DR, were also studied to interpret experiments and to test the DR theory. The plasma field and the density effects on the rate coefficients was found to be important, and a consistent correction procedure is being developed. The available data on the DR rates and their accuracy do not yet fully meet the requirement for plasma modeling; there are serious gaps in the available data, and the currently adopted theoretical procedure needs improvements. Critical assessment of the current status of the DR problem is presented, and possible future work needed is summarized.

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1. Introductory Summary

This is the final progress report on the DOE supported research project on the 'atomic processes in high temperature fusion plasmas'. The principal objectives of this study were to analyze those atomic processes which are important in plasma modeling, and specifically to calculate the reaction cross sections for the resonant modes. The reaction rates were to be evaluated under the assumption of local thermal equilibrium. The major part of our effort was directed toward the rate evaluation for the dielectronic recombination (DR), which is a resonant mode of electron capture by ions forming a doubly excited state, which subsequently decays by x-ray emission. All the ions with all degrees of ionization which may be present in a fusion plasma must be treated theoretically. Since the amount of required computations is enormous even with the simplest procedures, such as the distorted-wave Born approximation, it was necessary to limit the calculation to a small set of isoelectronic sequences. The result thus obtained are then used as benchmarks in constructing a simple interpolating empirical formula for DR, which may be used for plasma modeling to generate very quickly all the DR rates that are needed as inputs to the rate equations.

The DR rates are also needed in plasma diagnostics, where the intensity and the energies of the x-rays emitted by the plasma are analyzed to obtain information on the local conditions of the plasma; both spatial and temporal distributions of ions and their composition, temperature etc. However, the accuracy requirements on the rate data can be different for the above two general purposes, plasma modeling and plasma diagnostics. For modeling, a complete set of rates is needed as an input to the rate equations that represent all ions which are present in a plasma, with all degrees of ionization. Obviously, the needed rates cannot be calculated explicitly with high accuracy, because of computer and

man-power limitations; generation of the DR rates for one ion of nuclear core charge Z_c and the degree of the initial ionization Z_i may take a minimum of three to six months of a trained physicist, working full-time. Therefore, the accepted procedure is to calculate the rates for a small number of key ions as benchmarks. With proper parametrization, ~~the~~^{the} ~~rate~~ formula provides interpolation to other ions and could very quickly generate the needed rates for any ions of interest. The currently targeted accuracy is at the 20-30% level. On the other hand, in the plasma diagnostics, ~~the~~ rates of much higher accuracy are generally desired, perhaps at the level of 5 to 10 % . Such accuracy is often feasible theoretically since the number of charge states to be treated is limited. Many important corrections have to be included to attain such high accuracy. These two tasks are mutually inclusive; the high accuracy data for plasma diagnostics provide spot checks on the crude data base for modeling, while a large quantity of data for modeling is often useful in determining the overall trends and pointing out where improvements could be made.

The calculation of the DR rates is a complicated, intricate and often tedious theoretical task, and requires roughly one to two man-years to generate the rates for one complete isoelectronic sequence, so long as the number of electrons in the ions is not too large ($N \lesssim 10$). There are thousands of resonance levels to consider and a large part of them is treated individually. Their contributions are then summed over at the end to get the total rates. Many approximations have to be introduced, some of which are tested for their validity but some others are adopted for convenience. There are essentially two types of initial excitation modes during the capture process, the intershell ($\Delta n > 0$) and intrashell ($\Delta n = 0$) excitations. The former usually involves hard collisions with large excitation energies, while the latter is a soft collision with small excitation energies and ac-

accompanied by a capture of the incoming electron to high Rydberg states ($n \gg 1$). It turned out that these two modes have rather distinct dependence on N , T , and $n \gg 1$. This point is later exploited in constructing the rate formula. The theoretical procedure has to be examined and improved on a continuing basis in order to meet the new situations and elevated requirements. Several other groups, notably NLL and ORNL, joined in this effort. Unfortunately, in spite of the strenuous effort, the task of generating the complete set of DR rates for all ions that meet the modeling requirements is far from complete. However, compared with the situation ten years ago, we have made a great stride toward this objective. An order of magnitude larger data base is now available. But more importantly, we now understand better the intricacies of the resonant processes as they are affected by the plasma environment where the reactions take place.

During the course of the DR rate evaluation for the last 12 years, experimental efforts by a number of groups produced the DR cross sections. Some other reaction data that are related to DR were also reported. Thus, all the direct electron-ion cross beam and the merged beam experiments involved the soft-collision type, $\Delta n = 0$. The cross sections were very sensitive to external electric fields which were present in the interaction region. The perturbation was very strong because of the presence of high Rydberg state electrons, and the cross sections were drastically enhanced, sometimes as much as a factor of five. This important finding triggered much research activities during the past seven years. On the other hand, the hard collision mode of DR has been studied successfully experimentally through the ion-atom (and ion-molecular) collisions, where the target atom provided the 'electron beam' in the projectile ion rest frame, in the impulse picture. This resonant-transfer-excitation followed by x-ray emission (RTEX) was analyzed in a number of cases in terms of the folded DR cross

sections, with good agreement between experiments and theory. Unfortunately, no direct experiments are available on the electron-ion collisional DR for the $\Delta n > 0$ mode and the RTEX measurements on the $\Delta n = 0$ mode.

It has been stressed in the past that the various resonance processes in electron-ion collisions are inter-related, because of the factorization property of the resonance amplitudes, together with the impulse picture, the time-reversal invariance, and unitarity. Thus, the resonant modes of collisional excitation, ionization and capture are expressed by the same theoretical components (the Auger and x-ray transition probabilities). The photon-initiated resonance mode can also be related to DR by detailed balance. This inter-relationship has a profound effect on the DR study; (i) the various reaction data can be cross-checked, (ii) the cross sections for one reaction may be converted to that of another.

In this report, we will summarize the work we completed, with a critical assessment of the data available. Several key areas which are yet to be studied are pointed out.

2. Work Completed on DR.

2.1. The DR rate calculation

The following isoelectronic sequences have been treated by the UConn group during the past twelve years:

$$N = 1, 2, 3, 4, 10, 11 \text{ and } (5, 9, 12)$$

for ions with the number of electrons N before capture, and the numbers in the parenthesis indicate that the available data are only partial. The contributions of other groups involve the sequences $N = 1, 2, 3, 4, 9$ and 10 . Our calculations were in most cases the earliest ones reported, and the later calculations by the other groups are usually checked against our result. In many cases, the agreement was satisfactory, while the new calculations sometimes extended and/or improved them.

A new and improved empirical formula is being generated that reproduces all the existing data, and interpolates to all ions with $N \lesssim 13$ and $Z_c \lesssim 40$. A preprint of the paper on this work is attached. We have been only partially successful in this task for the following reasons: i) Much of the data are not complete, ii) accuracy of the data is not uniform and their assessment is difficult, and iii) for fitting and interpolation purposes a minimum number of parameters must be introduced that may distort the result. Obviously, the result we have obtained is far from definitive, and requires further updating on a periodic basis as more data become available.

2.2. DR cross sections.

Both the $\Delta n = 0$ and $\Delta n > 0$ modes of DR cross sections have been computed for a selected set of ions, and the result compared with both the direct DR and RTEEX experiments. In addition, the same theoretical code was used to generate

the resonance excitation and resonance ionization cross sections, for comparison with experimental data. In all cases the agreement between theory and experiments was satisfactory.

2.3. Plasma density and field effects.

The electric field effect on the DR rates has been extensively discussed since 1982, and we have now a reasonably good understanding of this effect. However, there exist some discrepancies in the state distribution of the DR products, which are yet to be clarified. The plasma density effect caused by the collision of the captured high Rydberg state electrons with the plasma electrons is only beginning to be understood. The n and ℓ changing collisions for the densely populated resonance levels have to be properly treated. Furthermore, it should be emphasized that the field and density effects are not independent of each other, and eventually they have to be treated simultaneously.

3. Milestones Achieved

The following milestones have been achieved during the past ten years by the University of Connecticut atomic theory group:

a. Electron-ion collisions:

1. Ionization.

- The importance of the resonant mode of ionization was first suggested by a sum-rule type calculation (PRL 39, 82 (1977)).
- A higher-order resonant mode, REDA, was proposed, and a distorted wave calculation was performed (refs. 8 and 11)

2. Excitation.

- The serious omission in the study of x-ray lasing reaction of the resonant mode of excitation in $\text{Se}(24+)$ was pointed out. (ref.54)

3. Recombination.

- The first calculation of the dielectronic recombination cross section for $\text{Cl}(7+)$, $\text{Mg}(+)$ and $\text{C}(+)$ was performed, and the result compared with experiments (refs. 16, 19, 24).
- Many large-scale computation of the dielectronic recombination (DR) rates for plasma modelling have been performed (refs.1-7, 37, 59)
- Some high accuracy calculations of the DR cross sections were carried out, for comparison with experiments (refs. 63, 65, 71, 77, 79).

4. Electric field effect.

- The role of the electric field in dielectronic recombination of Mg was proposed and a theoretical estimate obtained which was in agreement with experiment (refs. 26, 39, 47, 48, 30)
- The effect of electric field rotation on the DR cross section was examined and the discrepancy in the state distribution pointed

out (ref.46)

b. Ion-atom collisions:

1. RTEX-resonant transfer excitation followed by x-ray emission. Some of the earliest calculations of the DR cross sections were performed here to analyze experiments, by folding the cross section over the target Compton profile. (refs. 13, 56, 57, 66).
2. RTEA-RTE followed by Auger electron emission. The first analysis for $O(5+)$ was performed (ref.41)
3. NTEX-nonresonant TEX. The first realistic calculation of the cross section was performed for $S(13+)$ and explained the experiment (ref.67)
4. UTEX-uncorrelated TEX. The presence of this mode was suggested, and recent ORNL experiments on F and Berkeley experiments on Nb seem to show its existence. (ref.69)

c. Photo-ionization:

Several initial estimates were made on the contribution of the resonant mode of photoionization rates. A radiative-Auger cascade model is applied to study the final charge distribution in the decay of inner-shell vacancies. (refs.14, 81, 78).

d. Review articles:

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2. Physics Reports, 166, 195 (1988). with K. LaGattuta
3. Comments on Atom. Molec. Phys. 13, 103 (1983)
4. Comments on Atom. Molec. Phys. 19, 99 (1987)
5. Physica Scripta T28, 25 (1989)
6. Physica Scripta, T37, 53 (1991)d.

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5. Training of students

The number of atomic theorists trained : 14

a. Postdocs:

Dr. J. Gau (1977-79).

Dr. K. LaGattuta (1979-85),

Dr. M. Janjusevic (1986-88)

b. PhD's:

Dr. D. McLaughlin (1983),

Dr. I. Nasser (1985),

Dr. G. Omar (1987),

Dr. H. Ramadan (1989).

c. Training of faculties and students:

Dr. Ali Moussa,

Dr. M. Dube,

Dr. N. Shkolnik,

Dr. R. Rasoanaivo,

Dr. J. Retter,

R. Luddy

R. Bellantone,

6. Critical Assessment of the Project

6.1. Lack of DR rates for $N \gtrsim 12$. In spite of the long and arduous efforts, the necessary information on DR for the completion of constructing a rate formula is insufficient. The ions with large number of electrons can be present near the cooler plasma edges, and, for heavier impurity ions such as Mo and W, even in the interior regions. The theoretical calculation of the DR rates and the related resonant modes is more difficult for ions with $N > 10$, because of the higher density of excited levels. The configuration interaction between a large number of levels becomes more important, and the conventional procedure in which the individual levels are treated separately is no longer effective. In addition, some of the higher-order processes which have been neglected thus far for the low N ions may become significant. At present, no viable theoretical procedure exists, and no significant progress could be achieved until a more effective theoretical procedure is found and tested. The data gap for ions with $N > 11$ is one of the more serious shortcomings of the current status.

6.2. An additional gap in the available DR rates exists for ions with N in the range $4 < N < 10$. There are already indications of complexity in these ions that we would expect only for the $N > 10$ cases; the two excitation modes discussed in sec. 2 are no longer distinct as N approaches $N = 10$, so that it is not possible to treat them separately to reduce the complexity of the calculation. Some scattered data are beginning to be available for $N = 5$ and 9, but much more work is needed to fill this gap.

6.3. Accuracy assessment. The calculations of the rates were carried out by different groups, and the approximations adopted were not the same. As a result, the reliability of the results obtained is not all uniform, and it is often very diffi-

cult to make a correct assessment of the accuracy. This, together with the lack of data, is a serious problem in generating a useful empirical formula.

6.4. The most serious from the practical point of modeling is inclusion of the effects of plasma density and field into the rate calculation. To make the matters worse, this problem is also linked to a particular way the rate equations are set up; the effect of the states which are truncated in the rate equations should be incorporated in the rate coefficients. Thus far, no systematic corrections have been included in the rates and in the empirical formulas. Since the effects could be very large, the accuracy requirement on the final rate coefficients must reflect this uncertainty as well. The extent to which the rate calculation should be pushed has to be critically re-examined.

7. Conclusions

Much progress has been made during this project period in the calculation of the DR rates and understanding the various theoretical procedures to be used. The effects of plasma environment on the rates are beginning to be clarified as well. But, much more work is yet to be done.

7.1. A new method of calculating the rates is needed for ions with more than ten electrons, where there are excessively large number of resonances, which are closely spaced and mutually interacting. The currently available approaches are not effective and too cumbersome at best. As a result, no data are available for ions with $N > 12$.

7.2. Almost all the cases studied involve ions in the ground state configurations. This is of course not sufficient in a more realistic situations inside the tokamak plasma, at high temperature. The data for the excited states are needed both in modeling and in diagnostics, specially those involving intra-shell excitations with relatively small excitation energies.

7.3. As noted above in Sec. 6, the most important problem to be resolved is the effect of the plasma field and density. It can be as much as a factor of ten change in the rates. No applicable theoretical procedures are available.

7.4. The strong electron correlations in the case of doubly excited Rydberg states must be treated more carefully, since the usual central field classification of these states breaks down. Furthermore, due to the same correlations, processes involving more than two electrons are possible, such as the shake-off. These effects are either ignored completely, or treated crudely, as no reliable methods are available.

7.5. The plasma environment in which atomic processes take place is often turbulent and far from thermal equilibrium. The Maxwell distribution assumed for

the electrons may not be valid, and the temperature in LTE is ill-defined. In such cases, the rates as we ordinarily define are meaningless.

For all the above reasons, each of which is serious on its own right, there are still much more work to be done in understanding the atomic processes in high temperature plasmas. The above remarks presumably also apply to other resonant processes, such as the excitation-autoionization and resonant excitations.

8. Reprints and Preprints Attached.

1. Physics Scripta, T28, 25 (1989)
2. Physica Scripta, T37, 53 (1991)
3. Improved DR rate formula (preprint)
4. Plasma density and field effects on radiative recombination
5. Physica Reports. 166, 195 (1988)

*Reprints removed and
cycled separately.*

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