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Theory of dielectronic recombination and plasma effects

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Abstract: Current status of the various theoretical approaches to calculation of dielectronic recombination rates is summarized, with emphasis on the available data base and on the plasma effects of both the plasma ion (and external) fields andplasma electron collisional effects which seriously affect the rates and complicate compilation of data.

1. Introduction. Dielectronic recombination (DR) is one of the three known ways by which plasma electrons recombine with ions. The other two are the radiative recombination (RR) and three-body recombination (TBR). In all cases, the excess energy is released by the recombining electrons, and carried away by emitted photons in RR, by increased kinetic energy of the participating electrons in TBR, and in DR by one of the bound electrons as it is excited to form a multiply excited states of ions. The DR process was first suggested in the 1940's by Bates and Massey in connection with the astrophysical problems, and later its importance was recognized by Burgess. The realization in the 1970's, that the DR by impurity ions in tokamak was the dominant cooling mechanism, was probably the main incentive for much of the research activities since then, both experimentally and theoretically. For highly charged impurity ions in high temperature plasmas, heavy-ion accelerators with storate rings and EBIT have played a specially important role in generating experimental data, while for low-charged ions large effects of electric fields on DR rates were observed. There have been several reviews on the subject recently [1,2], so only a couple of pertinent points will be made; the 1992 reviews by the experts in the field, both experimental and theoretical, provides an excellent basis of reference.

a) Modelling of high T plasmas requires a complete set of DR rates, in addition to many other rates for the processes that are taking place. Most of the reactions involved are the topics of this workshop. But, inspite of much efforts of the past 30 years, the available data are far from complete. Besides, almost all data are for the initial ground states of ions.

b) At relatively low temperature, the plasma field and collisional effects can be important. Only a handful of cases have been analyzed, and no systematic compilation of data is currently possible. (See section 3 for further discussion).

In the simplified independent electron picture, the DR is a two-step process of excitation/capture, followed by a radiative decay to Auger stable final states. It is schematically described by

$$e_1^- + (e_2^- + A^{Z+1})_g \rightarrow [e_{1b}^{-\prime} + (e_2^- + A^{Z+1})_a]_{d=a+b}$$
$$\rightarrow (A^{Z-1+})_f^{\times} + x$$

where g = ground state ($n_g\ell_g$) of the target ion with charge Z, a = excited intermediate state of the target with $n_a\ell_a$, d = compound doubly excited states of the recombined ion of charge Z-1 and ($n_a n_b$), and f = final state of the recombined ion in a singly excited state with ($n_f = n_b$). x = emitted radiation. The excitation energy $\Delta_{ag} = E_a - E_g$ is supplied by the recombining electron, as $\Delta_{cb} = E_c - E_b = \Delta_{ag}$. This makes the DR a resonant process with sharp dependence on the continuum electron energy E_c.

It has been found convenient to categorize the DR process into three groups based on the different modes of excitation, although this separation becomes less clearcut as the number of open-shell electrons increases. We have, with $\Delta n \equiv n_a - n_g$ and $\Delta \ell \equiv \ell_a - \ell_g$,

(i) $\Delta n \neq 0$ involving inter-shell transitions with Δ_{ag} large and n_b small.

(ii) $\Delta n = 0$, $\Delta \ell \neq 0$ involving intra-shell transitions with Δ_{ag} and n_b of mederate size.

(iii) $\Delta n = 0$, $\Delta \ell = 0$, involving inter-multiplet transitions, with small Δ_{ag}, large n_b.

The doubly excited states (d) formed by the initial step of excitation-capture in the DR process are affected by the plasma effects, due to the plasma microfield of the plasma ions as well as any externally imposed electric and magnetic fields, and also the collisional effects of plasma electrons. We denote them as plasma field distortions (PFD) and plasma collisional transitions (PCT), respectively. These two effects are not additive, however, and must be included in modelling of the plasma in a consistent way, without double counting. The outer-shell electrons in state (d) with the principal quantum number n_b are in HRS for the excitation modes (ii) and (iii), and thus are most affected by the plasma effects.

2. The DR theories. Most of the data on the DR rates available thus far have been generated by a variety of theoretical methods, with varying degrees of accuracy. Since the work involved in the calculation of the rates is often complex and time consuming, much efforts have been expended to developing procedures that are suited for each specific purpose, and many extensive computer codes are available.

The DR rates and cross sections involve basically two building blocks, the autoionization and radiative decay probabilities, defined as $A_a(d_1 d_2 \rightarrow c, g) = 2\pi| < d_1 d_2 | V_{12} | c, g > |^2$, and $A_r(a \rightarrow f) = 2\pi| < f | \varepsilon \cdot \vec{r} | a > |^2$, respectively. Then, for example in the isolated resonance approximation, where overlapping resonances term are neglected, the DR rates are given by

$$\sum_d \alpha^{DR}(i \rightarrow d \rightarrow f) = (4\pi Ryd/k_B T_e)^{3/2} \sum_d (g_d/2g_i) \exp(-e_c(d)/k_B T_e) \; A_a \Gamma_r / (\Gamma_a + \Gamma_r)$$

where $\Gamma_r(d) = \sum A_r(d \rightarrow f)$ and $\Gamma_a(d) = \sum A_a(d \rightarrow j)$. Thus, accurate α can be constructed once reliable A_a^j and A_r are available, which in turn depend critically on the various electronic wave functions involved in the A's. Theoretical methods employed may be summarized, in the order of increasing complexity and accuracy:

1) Scaled coulomb approximation with effective Z and quantum defects. The calculation can be analytic, and the approach is especially suited in treating high Rydberg state electrons and high Z ions. The overall behavior in Z, n, and T can then readily be inferred. But, the method is less accurate when high precision is sought.

2) Non-relativisitc distorted wave method for the continuum orbitals and model potential (or Hartree-Fock) bound state orbitals in the evaluation of A_r and A_a. Various angular momentum coupling schemes are available, such as LSJ, jjJ, and jK, etc. Some relativistic effects may be included perhaps for Z < 30, and cofiguration mixing can be incorporated.

3) Close coupling/ R-marix method for the continuum orbitals, and a set of model wave functions for the bound orbitals. For light ions, this is probably the most accurate approach, but involves many complex steps and often can be very time-consuming [3 – 5].

4) Relativistic distorted wave method, which is suited for treating highly stripped ions, especially for $Z > 20$, where the coulomb field is strong. Configuration mixing can improve the data.

3. Plasma effects - rate equations and rates. By the plasma effects, we mean a) the collisional effect of the central ion with the plasma electrons (PCT) and b) distortions of the electron orbitals (both bound and continuum) around the central ion by both the plasma microfield due to the plasma ions and externally imposed electric and magnetic fields (PFD). Generally, these effects can be incorporated either in the rates themselves or in the rate equations. But the rate equations are convenient in handling the collision effect, while the rates can readily handle the field effects.

3a. PFD. The static ion microfield is represented for example by the Holtzmark field, and its refinements can be made. Given the field, its effect on DR may be estimated by a simple 'full mixing' picture, where the spherical states are transformed to the stark states, via Clebsch-Gordan coefficients. However, this procedure does not depend on the field strength. A refined procedure is possible, in which a field-dependent phase factor is introduced. A more ambitious treatment involves diagonalization of the energy matrix that contains field shifts. For the excitation modes (ii) and (iii), experiments with light ions indicated that the change in the DR rates due to external electric fieldperturbation can be very large, increasing the rates by as much as a factor of ten. Theoretical analyses showed that such an enhancement is due to strong ℓ mixing with consequent redistribution of the Auger probability A_a relative to the dominant radiative probability A_r. In the simplest picture, this reduces purely to a state counting, in the spherical basis vs the stark (parabolic) bases.

In addition to the electric field effect, a magnetic field plus electric field can further modify the above result [6]; this case may be viewed as producing extra electric field in the Lorentz transformed drift frame with velocity $\vec{u} = c\vec{E}x\vec{B}/E^2$, with the change in the electric field of $\Delta\vec{E} = B^2\vec{E}/2E^2$.

3b. PCT. As noted, the PCT effect can be naturally included by employing the rate equations, which are usually truncated. On the other hand, it is possible to include the correction to this truncation in the rates a part of the collision effect in the rates by using a specially taylored Fokker-Planck operator, as $\tilde{\alpha}$ may be obtained by $\tilde{\alpha}^{DR}(m) \equiv [1 + \Omega]\, \alpha^{DR}(m)$, where Ω depends on the structure of the rate equations and rates. We have made some systematic study of the plasma collisional and field effects, for a simplified hydrogen plasma with carbon impurities [2].

4. DR rates - available data. In the study of high temperature astrophysical and laboratory plasmas, the DR rates are needed (A) for analyses of spectral lines emitted by impurity ions and (B) for modelling of plasmas to determine the ionization balance. Object (A) requires a small set of data of high accuracy, while (B) needs a large set of rates, which are presumably of less accuracy for practical reasons of difficulty in generating them. In 1989, a summary of the available DR data was given [7] for the Fe ions with the degree of ionization $Z = 1$ to 25. Except for a couple of regions of Z values where data existed, often with poor accuracy, much was not known. In 1993, the overall DR rates were summarized [7], in the form of empirical fitted formula, and poor status of the situation was pointed out. Since then some more high quality data became available, and Very little improvements have been seen since, but where there are new data, the fitted values have been improved, in some cases as much as an order of magnitude. As have been done previously, the rates were summarized in the form of empirical fitted formulas, but separately for each excitation modes discussed above. Only

the contribution from the excitation modes (i) and (ii) were considered. Mode (iii) is important only at low temperature, but the problem of field mixing can be serious.)
We emphasize several important points:
1. Almost all the data are for the target ions initially in their ground states. When these rates are used in the rate equation for modelling purposes, the DR from some of the long-lived excited states may be needed.
2. The rates are calculated routinely with the final (singly excite) states summed, so long as they are Auger stable; otherwise, the cascade effect must be included, that reduces the rates. This is in principle inconsistent with the rate equations to which they are applied.
3. As noted earlier, the contribution from excitation mode iii is usually not included in the empirical formulas. This must be rectified, with careful consideration of possible external field perturbations.

5. Summary. We have made three points of some importance in dealing with the DR processes in high temperature plasmas:

1. A more careful and consistent treatment is needed in defining the rates as they are used in a particular set of rate equations. This is especially relevant as to the way residual plasma collisional effect is to be included.

2. The DR data are much to be generated, with proper accuracy assessment, and adjusted to specific usage. The DR from the initial excited states are desirable, and the total rates, summed over all the singly excited final states, must be used with caution.

3. The DR rates associated with the excitation modes (ii) and (iii) are especially sensitive to external field perturbations, but nothing has been done. In view of large numerical efforts required in generating these rates, it is desirable to determine how the production and compilation can be systematized.

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