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CHARGE EXCHANGE AS A RECOMBINATION MECHANISM IN HIGH-TEMPERATURE PLASMAS

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Charge Exchange as a Recombination Mechanism
in High-Temperature Plasmas

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ABSTRACT

Charge exchange with neutral hydrogen is examined as a recombination mechanism for multi-charged impurity ions present in high-temperature fusion plasmas. At sufficiently low electron densities, fluxes of atomic hydrogen produced by either the injection of neutral heating beams or the background of 'thermal' neutrals can yield an important or even dominant recombination process for such ions. Equilibrium results are given for selected impurity elements showing the altered ionization balance and radiative cooling rate produced by the presence of various neutral populations. A notable result is that the stripping of impurities to relatively non-radiative ionization states with increasing electron temperature can be postponed or entirely prevented by the application of intense neutral beam heating power. A time dependent calculation modelling the behavior of iron in recent PLT tokamak high power neutral beam heating experiments is also presented.

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I. INTRODUCTION

Interest in the process of charge exchange between neutral hydrogen beams and multi-charged impurity ions

was initially stimulated by concern over its possible contribution to the premature deposition of the neutral beam particles in the plasma periphery (Girard, et al. 1975, Post, et al. 1976, Duchs, et al. 1977).

More recently, the effect of these charge exchanges on the impurity ions themselves has been recognized by the selective population of excited levels in oxygen (Isler and Crume 1978). Charge exchange induced recombination has also been observed as an important process for oxygen in the 2XIIB mirror device (Drake and Moos 1979) and calculated to be important for iron in the PLT tokamak (Hulse, et al. 1979a).

Our purpose here is to undertake a more general examination of the role of charge exchange induced recombination in determining impurity behavior in fusion plasmas, and to draw attention to its importance. To this end, charge exchange has been included in a zero-dimensional, time independent (coronal equilibrium) atomic physics code, as described in Section II. Results from this code for the altered ionization balance and radiative loss rates of selected impurity elements are given in Section III. Emphasis is given to highly charged ions present in

high temperature, low density neutral beam heated plasmas. The process is shown to play a particularly significant role in the physics of impurity behavior under these conditions, acting to maintain impurities in highly radiative charge states to extremely high electron temperatures. The relevance of this effect to current experiments is further demonstrated in Section IV, where a time dependent calculation is presented simulating the behavior of iron in the core of a PLT tokamak plasma during neutral beam injection. Final conclusions are given in Section V.

II. RATE COEFFICIENTS AND CROSS SECTIONS

1. Electron-Ion Processes

Transition rates for the electron-ion processes of ionization, recombination and excitation are calculated using generalized formulae essentially identical to those first developed for the 'XSNQ' average ion model code (Post, et al. 1977). These formulae are used in the present multi-species code to yield rate coefficients for each ionic species of an arbitrary element present in a low density, transparent (i.e., coronal) plasma of given electron temperature and density. The coronal equilibrium results for the average charge and overall radiation rate of an impurity calculated with this new code compare well with those from the earlier average ion code referenced above, with the present multi-species formulation providing a more

complete and physically straightforward basis for impurity studies such as the one described here.

For each ionic species of the element under consideration, energy levels are determined for the first ten principal quantum number (n) shells using shielding constants (Mayer 1947). Oscillator strengths and transition energies are computed for $\Delta n \neq 0$ transitions between these levels. $\Delta n = 0$ transitions are modelled using tabulated fitting parameters for a single 'equivalent' $\Delta n = 0$ transition oscillator strength and transition energy for each species. The electron collisional ionization, radiative recombination, and dielectronic recombination rates are then calculated for each species using the relevant oscillator strengths and energies along with the specified plasma electron temperature, T_e , and electron density, n_e . Similarly, radiation rates are computed for each ionic species, including excitation of $\Delta n = 0$ and $\Delta n \neq 0$ line transitions, radiation associated with the recombination processes, and bremsstrahlung.

Ionization balances and total radiation rates are calculated from the rate coefficients by solving either the time independent (coronal equilibrium) or time dependent zero-dimensional, multi-species coupled rate equations.

2. Atom-Ion and Ion-Ion Processes

The recombination rate of an impurity ion of charge q due to charge exchange with a monoenergetic beam of hydrogen neutrals of velocity v_n cm/s and local density n_n cm⁻³ is given by

(2)

$$R_q^{CX} = n_n \alpha_q^{CX} = n_n v_n \sigma_{CX}(v_n, q)$$

where $\sigma_{CX}(v, q)$ is the velocity and charge dependent charge exchange cross section. For heavy impurity ions we need make no distinction between the relative interaction velocity v_{rel} and the beam velocity v_n , since we typically have $v_n \gg v_{th}$, the thermal velocity of the impurity ions.

Cross sections for charge transfer from neutral hydrogen to fully stripped impurity ions have been taken from three theoretical calculations in the literature. Olson and Salop have calculated these cross sections for low relative velocities ($v < 1 \times 10^8$ cm/s) using an absorbing sphere model (Olson and Salop 1976, hereafter referred to as OSAS), and for high velocities ($v > 2.7 \times 10^8$ cm/s) using a classical trajectory approach (Olson and Salop 1977, denoted by OSCT). These results, plus those from a tunneling model due to Grozdanov and Janev (1978, denoted by GJ) have been approximately fitted and used in the code. For 40 keV deuterium beams (such as those used on the PLT tokamak), we have 20 keV/amu or a velocity of $v_n = 2 \times 10^8$ cm/s. This is unfortunately near a characteristic velocity of the interaction (the Bohr Velocity, 2.2×10^8 cm/s), which is reflected in the tendency of the theoretical calculations to avoid this velocity range. Figure 1 shows the adopted cross sections as a function of ionic charge. For $v = 2 \times 10^8$ cm/s curves are shown for GJ and for the appropriate limiting velocities of OSAS and OSCT. Also shown are the OSAS cross section for $v = 2 \times 10^7$ cm/s (indicative of the value for 400 eV

thermal deuterium neutrals) and the OSCT values for $v = 3.5 \times 10^8$ cm/s (corresponding to the 60 keV/amu beams planned for the TFTR tokamak).

Despite different velocities and theoretical methods, the curves in Fig. 1 are all quite similar, particularly for highly charged ions. More recent theoretical calculations for Fe^{+26} (Salop and Olson 1979) and other ions (Ryufuku and Watanabe 1979) continue to yield reasonable agreement with the values shown. Experimentally, existing high-velocity data are in reasonable agreement with OSCT (Berkner, et al. 1978, see also OSCT). At lower velocities, however, recent experiments using multiply charged Xenon indicate that the corresponding OSAS and GJ results may somewhat over-estimate σ_{cx} (Crandall, et al. 1979). Current experimental work is beginning to cover the wide range of charge states and velocities of potential interest for charge exchange recombination studies, although much further work clearly needs to be done.

While remaining uncertainties in the value of σ_{cx} provide a problem for very detailed calculations, it seems clear that σ_{cx} is sufficiently well known to support the general survey of charge exchange recombination effects presented in the following sections. Since σ_{cx} enters only as a product with n_n , the neutral density, the effect of an overall multiplicative uncertainty in σ_{cx} can be readily gauged in the time independent results by a compensating variation in n_n . We will adopt the OSCT values for beam interaction velocities, using the limiting $v = 2.7 \times 10^8$ cm/s values for the $v_n = 2 \times 10^8$ cm/s (20 keV/amu)

case. These are the most conservative (smallest) values for σ_{cx} at this velocity. The larger GJ values are used along with these OSCT values in Section IV as a test of the sensitivity of the time dependent calculation to the adopted σ_{cx} . The OSAS values are used for the $v_n = 2 \times 10^7$ cm/s thermal neutrals calculations.

These cross sections are formally computed for interactions with fully stripped ions of charge Z . For partially stripped ions the cross section corresponding to $Z = q$, the net charge of the ion, will be used. This is a good approximation for the multiply charged states of interest in the present calculations, as the capture occurs at relatively large distances from such ions into a shell of high principal quantum number n (OSAS, GJ, OSCT, Salop 1979, Ryufuku and Watanabe 1979).

Since the recombining electron is left in a highly excited (Rydberg) state for highly charged ions, we must consider whether collisional ionization and/or excitation out of this state is likely to interrupt the recombination process before decay to the ground state is complete. An estimate of this effect was made using a result by Wilson (1962) for n_t , the principal quantum number corresponding to the thermal limit at which collisional excitation and ionization rates balance the collisional de-excitation and radiative decay processes. Charge transfer proceeding into levels with $n > n_t$ will thus fail to result in ground state recombined ions, and the effective charge exchange recombination rate would need to be reduced proportionately. As an estimate for n_{cx} , the average n level for the captured electron, we use simply $n_{cx} \leq q$, the ionic charge (Olson 1979,

OSAS, Salop 1979, Ryufuku and Watanabe 1979). This corresponds to quasi-resonant (or deeper) capture, e.g. into levels with ionization potentials $I_p \geq 13.6\text{eV}$. We find that for plasmas of interest ($n_e \leq 10^{15} \text{ cm}^{-3}$) we have $n_{cx} \leq q < n_t$, and thus no collisional interruption factor is used in the present calculations. The strong $n^{-9/2}$ dependence of the radiative recombination rate (Griem 1964) assures that interruption becomes negligible very quickly for $n_{cx} < n_t$. A final caveat concerns the tendency of charge exchange to selectively populate high angular momentum (ℓ) states (Salop 1979, Ryufuku and Watanabe 1979). Such a non-statistical distribution would require re-calculation of the Wilson n_t result, except that ℓ -changing collisions for such Rydberg states are extremely rapid at these densities (Pengelley and Seaton 1964). These collisions will serve to quickly establish the usual statistical distribution of states before any collisional or radiative $\Delta n \neq 0$ processes become important.

Also calculated is the radiation rate due directly to the recombination cascade after each charge exchange capture. Since the recombining electron is typically left in a relatively high level with a binding energy much less than its final ground state binding energy, a full ionization potential of the recombined ion is presumed to be radiated for each charge exchange recombination event.

Proton impact ionization of the impurity ions has not been included. An estimate for this rate coefficient (Weisheit 1975) plus the assumption that $n_p \sim n_e$, $T_p \sim T_e$ indicates that it should

remain less than the corresponding electron rate for the temperatures considered here. If $T_p \gg T_e$, however, this process will tend to produce more ionized species distributions at the high-temperature extremes of the Section III results.

Ionization of the highly charged impurity ions by the neutral atoms is a negligible effect (Shirai, et al. 1977) and is not included.

III. EQUILIBRIUM RESULTS FOR HEAVY IONS

The transition rate per ion for the usual 2 - body, electron-ion processes of importance in coronal conditions are equal to the electron density, n_e , times a rate coefficient. With the exception of a weak density dependence for dielectronic recombination, these rate coefficients are themselves independent of n_e . The usual coronal equilibrium ionization balance, which is determined by ratios of the ionic rates, is thus virtually independent of n_e for the low densities typical of tokamak or mirror fusion plasmas ($n_e \leq 10^{15} \text{ cm}^{-3}$).

Charge exchange recombination, by contrast, is proportional to the neutral density n_n and independent of the local electron density. (The global electron density distribution in the device in question may of course play an indirect role in determining the rate of charge exchange recombination, by determining the penetration of neutrals into the plasma and hence n_n .)

In coronal equilibrium, we have the relative abundance of adjacent ionization states determined by the ratio of their total recombination and ionization rates per ion:

$$\frac{n_{q-1}}{n_q} = \frac{R_q}{I_{q-1}} = \frac{\alpha_q^{\text{RAD}} + \alpha_q^{\text{DIE}} + (n_n/n_e)\alpha_q^{\text{CX}}}{K_{q-1}} \quad (3)$$

where α_q^{RAD} and α_q^{DIE} are the radiative and dielectronic recombination rate coefficients, respectively, and K_q is the electron ionization rate coefficient. Thus, to the extent that coronal equilibrium results without charge exchange recombination are independent of n_e , the corresponding results with charge exchange recombination are a function only of n_n/n_e , the neutral fraction, for a given neutral velocity distribution.

As an initial illustrative case, we consider plasma parameters such as might be found just after the start of 40 keV neutral deuterium injection into a PLT low density discharge. At the plasma core, we have He-like Fe^{+24} as an important impurity ion, with $T_e \sim 2\text{keV}$ and $n_e \sim 2 \times 10^{13} \text{ cm}^{-3}$. The appropriate neutral density, $n_n \sim 1 \times 10^8 \text{ cm}^{-3}$, is found by taking the toroidal average of the spatially non-uniform density of beam neutrals seen by the rapidly moving impurity ion as it follows the field lines around the torus. Using OSCT cross sections, the resulting charge exchange recombination rates are readily found to be greater than the total electron-ion (radiative plus dielectronic) rates (Fig. 2).

Near temperatures of peak abundance in coronal equilibrium, radiative recombination is typically the dominant electron-ion recombination process for He-like, H-like, or fully stripped ions. The (mostly radiative) recombination rates of these ions are typically smaller than the (mostly dielectronic) recombination rates of lower charge state ions at their corresponding temperatures of abundance, making the highly stripped ions the most susceptible to added contributions. Furthermore, the charge exchange cross sections themselves are increasing functions of the ionic charge (Fig. 1). The impurity behavior is thus most sensitive to charge exchange recombination at temperatures where the highest ionization states are abundant. The coronal equilibrium species fractions for Fe, shown in Fig. 3 for varying amounts of neutral beam induced charge exchange, exhibit this characteristic behavior. With increasing n_n/n_e , the effect of the charge exchange process moves to progressively lower charge states and temperatures. Charge exchange induced enhancements of the total radiation rate from an impurity are primarily due to this shift of the ionization balance to less ionized (and thus typically more radiative) species distributions, rather than due to the direct recombination decay radiation occurring after each capture.

The slowly varying abundance curves seen at high temperatures in Fig. 3 for large n_n/n_e are the result of the relative insensitivity of the balancing electron collisional ionization rate to T_e in this region. At the highest temperatures shown, the system in fact begins to recombine with

increasing electron temperature as a consequence of having passed the peak of the ionization rate curves for these ions. As a test of the adequacy of the code's general ionization rate formula at these high temperatures, the ionization rate coefficient calculated by the code for Lithium - like Fe+23 has been compared with the more detailed result derived by Sampson and Golden (1978) (Fig. 4). The agreement is quite good, particularly in that the behavior at high T_e which produces the ionization balance stability and reversal appears in both curves. Also shown in Fig. 4 is the total K-shell excitation rate (as calculated by the code), which could potentially yield an autoionization contribution in addition to the direct ionization rate presently computed. However, even a unit branching ratio for autoionization would not appreciably alter the total rate, either in magnitude or in temperature dependence. Furthermore, for such highly charged ions radiative stabilization of such excitations will tend to dominate over autoionization.

Figures 5 through 8 show the equilibrium average charge state $\langle Z \rangle$ and total radiation rate coefficient ($P/n_e n_Z$, watts-cm³) for several elements as functions of T_e and the neutral fraction n_n/n_e . The curves are calculated for 20 keV/amu ($v_n = 2 \times 10^8$ cm/s), appropriate for the present 40 keV deuterium beams used on P.T. The OSCT cross sections are evaluated at their limiting velocity of $v = 2.7 \times 10^8$ cm/s. Since the variation of σ_{ex} with relative velocity is weak for the (high) charge states of greatest interest here (Olson and Salop 1977), the use of these values should not be a large source of error.

Similarly, curves for the 120 keV deuterium TFTR beams are not shown as the σ_{CX} for 60 keV/amu = 3.5×10^9 cm/s are only slightly smaller than the 20 keV/amu values for ions of primary interest (see Figure 1). The more energetic beam will, of course, have $(60/20)^{1/2} \sim 1.7$ times the flux for a given neutral density compared with the 20 keV/amu beam. This factor is somewhat offset by the smaller σ_{CX} , yielding an up to 60% larger 'effective' neutral density (depending on the charge states involved) to be used as an approximation for 60 keV/amu particles when using the 20 keV/amu curves. Similar approximations may be used for other beam energies and/or cross sections.

Figure 9 shows that 'thermal' background neutrals can also be effective in altering the ionization balance in low density plasmas. The calculation here used the same code as the beam cases, substituting for the beam velocity the average speed of the appropriate Maxwellian, in this case ($T_n = 400$ eV, deuterium) $\bar{v}_n = 2 \times 10^7$ cm/s. The corresponding OSAS cross sections were used (Figure 1). An illustrative situation for the center of a PLT low density ohmically heated discharge has this neutral temperature, $T_e \sim 1-2$ keV, and $n_n/n_e \sim 10^{-6}$.

IV. TIME DEPENDENT PLT MODEL

In order to evaluate non-equilibrium effects during intense neutral beam injection, the zero-dimensional time dependent code was used to calculate the behavior of iron impurity ions in the central region of a representative PLT discharge. The input

functions to this simulation are shown in Fig. (10a). Electron temperature and density data (Hinnov and Suckewer 1979) were used both directly by the multi-species code as shown and also as time dependent radial profiles input to a separate neutral beam deposition code. This latter code, FREYA (Lister, et al. 1976), was used to calculate the time dependent full, half, and third beam energy toroidally averaged beam neutral densities shown for 2.1 MW of parallel 40 keV deuterium injection. This zero-dimensional model does not include any impurity transport (diffusion), nor does it include any thermal background neutrals. Recent PLT experiments indicate that impurity transport effects associated with neutral beam injection must, in fact, be included along with charge exchange recombination if the iron behavior under such circumstances is to be fully understood (Suckewer 1979, Suckewer, et al. 1980, Hulse, et al. 1979b). The present model is thus intended only as an exercise to clarify the effect of charge exchange recombination alone, by assuming a simplified situation.

Figure 10b shows the calculated effect of the neutral beams on the Fe behavior, seen as a dramatic recombination of the impurity away from its original predominantly He-like charge state. Reference results are shown assuming $\sigma_{cx} = 0$, where the ionization distribution changes only slightly due to the imposed T_e change. The effect using $\sigma_{cx} = \text{OSCT}$ and $\sigma_{cx} = \text{GJ}$ are to be compared with the $\sigma_{cx} = 0$ curves. Results using the two different σ_{cx} are included as a measure of the sensitivity of

the calculated results to uncertainties in the theoretical cross sections.

The initially overwhelming effect of beam charge exchange recombination is attenuated by the rising plasma density as time progresses during the 150 ms beam pulse. This globally increasing density (due to beam fuelling) affects the critical n_n/n_e parameter by both sharply lowering beam penetration to the center as well as by directly increasing the local n_e .

V. CONCLUSIONS

Charge exchange between neutral hydrogen and multi-charged impurity ions is an important process which can significantly affect the behavior of such ions in high-temperature fusion plasmas. The effect on the ionization balance and radiative losses can be parameterized by the neutral fraction n_n/n_e for time-independent situations. The process can be of marked importance for both low and high Z impurities for values of n_n/n_e commonly attained in low density fusion plasmas. The source of these neutrals may be either neutral heating beams (including intermediate energy and thermal neutrals created by hydrogen-hydrogen charge exchange between the background ions and the beam), and/or the diffusion of neutrals from cooler regions of the plasma.

Emphasis was given here to moderately high Z impurities at high electron temperatures. Charge exchange recombination is first important for the most highly charged (He-like, H-like, and

fully stripped) ions. Near coronal equilibrium, the charge exchange process can most easily augment the relatively weak radiative recombination rates of these charge states. The charge exchange cross section, σ_{cx} , is also an increasing function of charge, contributing further to the vulnerability of the most highly charged states of the given element. At higher neutral fractions, lower charge states present at lower temperatures are also affected.

Significant charge exchange recombination is capable of maintaining relatively recombined ions at electron temperatures an order of magnitude or more above their ionization potentials. Rate coefficients for the usual electron-ion processes must, therefore, be evaluated far from their usual temperature regimes. Qualitatively new effects can result, such as ionization equilibria where the average ionization decreases with increasing electron temperature.

Inhibition of the usual 'burnout' (e.g., stripping) of heavy impurities to relatively non-radiative states with increasing electron temperature has serious consequences for plasmas dominated by power loss from such impurities. In such cases an anticipated breakthrough to dramatically lower losses via intense heating may prove futile, especially if the heating method of choice is neutral beams.

Unless n_i/n_e is known in advance to be negligibly small, charge exchange must be included along with the usual electron-ion impurity atomic physics and diffusion coefficients in order to achieve realistic results from impurity transport

code models. In particular, charge exchange may play an important role in resolving the commonly observed discrepancy between theoretical (especially coronal equilibrium) results for radial charge state distributions, and experimental observations of noticeably more recombined ions (Suckewer and Hinnov 1979). While charge exchange recombination will make elucidation of plasma transport effects from such observations somewhat more complex, it can also make traditionally difficult to observe fully stripped impurity ions amenable to study by the (transient) attachment of an electron during neutral beam injection. Line radiation produced by the resulting H-like ions has been shown adequate to allow measurement of the fully stripped ion abundance even at electron temperatures well above the highest ionization potential of the impurity element in question (Afrosimov, et al. 1975).

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FIGURE CAPTIONS

- Fig. 1. Adopted cross sections for charge exchange between a fully stripped ion of charge Z and neutral hydrogen atoms at selected velocities. OSAS, GJ, and OSCT label three different theoretical calculations (see text). The solid curves show σ_{CX} for the velocity closest to 2×10^8 cm/s (20keV/amu) for which each of the three calculations is valid.
- Fig. 2. The recombination rate of Helium-like Fe⁺²⁴ due to various densities of 20 keV/amu hydrogen neutrals, compared with the total radiative plus dielectronic rate as a function of T_e .
- Fig. 3. Ionic species abundances in neutral-beam modified 'coronal' equilibrium for iron as a function of electron temperature. Results are shown for four values of the neutral fraction n_n/n_e of 20 keV/amu hydrogen, using the OSCT cross sections.
- Fig. 4. Ionization rates for Lithium-like Fe⁺²³ as a function of electron temperature. The direct ionization rate calculated by the code compares favorably with the Sampson and Golden rate, even to high temperatures.

Any possible autoionization contribution due to K-shell excitations is small.

Fig. 5. Oxygen neutral-beam modified 'coronal' equilibria. Hydrogen neutrals at 20 keV/amu are considered, using the OSCT cross sections. The curves are parameterized by the neutral fraction n_n/n_e . Shown are (a) the average charge state $\langle Z \rangle$, and (b) the overall radiation rate coefficient $P/n_{e n_2}$, both as functions of the electron temperature.

Fig. 6. Titanium charge exchange equilibria (see Fig. 5).

Fig. 7. Iron charge exchange equilibria (see Fig. 5).

Fig. 8. Molybdenum charge exchange equilibria (see Fig. 5).

Fig. 9. Iron charge exchange equilibria for 200 eV/amu ('thermal') neutrals, using OSAS cross sections; otherwise, as for Fig. 5.

Fig. 10a. Input Functions for the zero-dimensional time dependent model of the effect of charge exchange recombination on iron impurity ions in the core of a 2.1 MW beam-heated PLT plasma.

Fig. 10b. Calculated result for the behavior of the iron impurity average charge $\langle Z \rangle$, Fe^{+23} abundance, and total radiation rate per ion using the Figure 10a input functions and either OSCT or GJ cross sections (see text).

Fig. 1 792656

Fig. 2 792657

Fig. 3a,b 792652

Fig. 3c,d 792651

Fig. 4 792654

Fig. 5 792578

Fig. 6 792576

Fig. 7 792653

Fig. 8 792575

Fig. 9 792572

Fig. 10a 792580

Fig. 10b 792655

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