Contribution of excited hydrogen atoms to charge-exchange excitation of impurities in fusion plasmas

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Cross sections are calculated for charge transfer into excited states of C^{5+} and O^{7+} from collisions of C^{6+} and O^{8+} with hydrogen atoms in the $n=2$ and 3 levels. Effective emission cross sections that account for cascading are then derived for spectral lines emitted when the product ions decay. These are compared to the emission cross sections calculated for excitation by ground-state hydrogen. It is shown that in some circumstances the contribution from excited hydrogen atoms must be taken into account when visible lines are used to determine the oxygen or carbon density from charge-exchange spectroscopy in plasmas. Influences on Lyman-series spectra in the x-ray region are also discussed.

Fully ionized carbon and oxygen are usually the dominant impurity species in high-temperature plasma devices.[1] Although these ions cannot be identified by electron excitation of characteristic spectral lines, they can be detected through lines emitted from the one-electron ions which are formed in excited states following charge transfer from atomic hydrogen:

$$C^{6+}+H(n_H)\rightarrow C^{5+}(n)+H^+ \quad (1)$$

and

$$O^{8+}+H(n_H)\rightarrow O^{7+}(n)+H^+ . \quad (2)$$

These charge-exchange excitation (CXE) lines have been used successfully to measure low-Z impurity concentrations in tokamaks by observing radiation emitted along the path of a neutral-hydrogen heating beam or diagnostic beam and relating spectral intensities to theoretical emission cross sections which include cascading.[2] Most experiments have utilized $\Delta n=1$ transitions from upper levels having $n\leq 5$ for which the emission cross sections are large, of the order of 10^{-15} cm^2, and which lie in the vacuum-ultraviolet region below 1000 Å. Strong interest is developing, however, in using transitions in the visible region which originate from more highly excited levels. The charge-transfer cross sections to these high-n levels from ground-state hydrogen can be two orders of magnitude smaller than those which dominate the production of the vacuum-ultraviolet lines, but the flexibility of utilizing transmission optics leads to much more convenient diagnostic systems. Moreover, in machines where large fluxes of neutrons are produced by fusion reactions, vacuum penetrations must be kept to a minimum, and it is desirable to exploit spectral lines that can be transmitted through windows or optical fibers.

Quantitative determinations of impurity densities from lines above 2000 Å entail certain complications that need not be considered for the $\Delta n=1$ vacuum-ultraviolet lines. Magnetic and electric fields and collisions can couple the nearly degenerate angular momentum states of high-n levels.[3,4] It is simple to account for such effects in the limit of complete statistical mixing, but accurate treatment is complex if only partial coupling occurs within an n level. Recent work on the Alcator tokamak at the Massachusetts Institute of Technology has suggested another possible complication, namely, excited hydrogen atoms in plasmas can disproportionately influence the intensities of lines from highly excited states of the charge-exchanged product ions.[5] The cross sections for transfer from excited atoms are much larger than those from the ground state,[6] so that even if the excited component is less than 1% of the beam current, it is not *a priori* obvi-

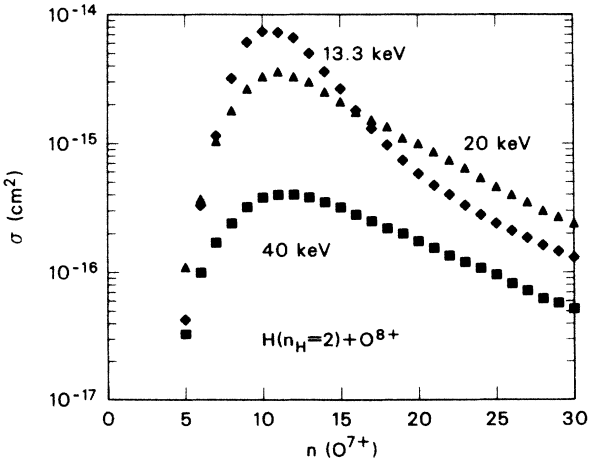

FIG. 1. Charge-transfer cross sections from hydrogen in the $n=2$ level to O^{8+}.

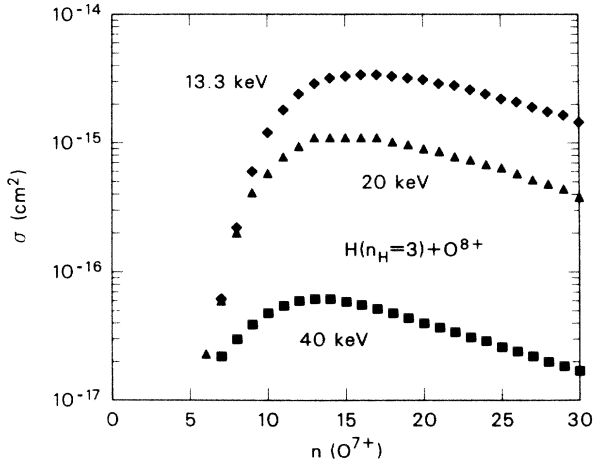

FIG. 2. Charge-transfer cross sections from hydrogen in the $n=3$ level to O^{8+}.

ous that its contribution to spectral excitation is negligible. At collision velocities, v_c, near the electron orbital velocity, $v_e=2.19\times10^8/n_H$ cm/s, where n_H is the occupied level of the hydrogen atom, the total electron-loss cross section is dominated by charge transfer and scales as n_H^4. At high velocities,[6] the electron-loss cross section (ionization plus charge exchange) scales as n_H^2/v_c^2. In this paper we investigate the influence of excited hydrogen on lines useful for charge-exchange spectroscopy of fusion plasmas. Charge-exchange cross sections are calculated into n levels ≤ 30 of C^{5+} and O^{7+} for incident hydrogen in the $n_H=2$ and 3 levels at energies of 40, 20, and 13.3 keV. These energies reflect the composition of the neutral beams employed for recent studies in the ASDEX tokamak at the Max-Planck Institute for Plasma Physics.[7] Effective emission cross sections, which include cascading, are compared for three different states of the hydrogen projectiles, and the contribution of the excited states to spectral line intensities are assessed for some typical plasma conditions.

The cross sections for charge transfer from the $n=2$ and 3 levels of hydrogen into excited levels C^{5+} and O^{7+} are computed by the classical trajectory Monte Carlo method.[8] This technique has been tested extensively for $1\leq v_c/v_e\leq 10$ and has been shown to yield accurate cross sections. For the cases addressed in this study, v_c/v_e ranges from 1.4–3.7. Since the electron tries to preserve its original energy and orbital dimension after capture, the levels most likely to be populated are those which satisfy the condition $n_H\sqrt{q}\leq n\leq n_H q$ with the maximum cross section occurring near the middle of the distribution.[6] This feature can be seen in the results illustrated in Figs. 1–4, but in most cases the cross sections are not sharply peaked at a single n level of the impurity ions. As expected from the $1/v_c$ scaling, excited beam atoms charge exchange more efficiently for the one-third- and one-half-energy components than for the full-energy component, so that excited states are less likely to be important for beams with a highly favorable species mix (i.e., dominantly constituted of the full-energy component). Figure 5 compares charge transfer to oxygen from ground-state and excited-state hydrogen. For $n=10$ and above the charge-exchange cross sections are more than two orders of magnitude greater for $n_H=2$ and 3 at 20 keV than for $n_H=1$ at 40 keV. Thus, when the beam current in the lower-energy components is comparable to that in the full-energy component, excited atoms cannot be disregarded if their concentrations are of the order of 1%.

Excited hydrogen-atom fractions are evaluated from the coupled rate equations which take account of collisional processes and radiative decays between levels up to the Lorentz ionization limit. Electron[9] and ion[10,11] excitation, de-excitation, and ionization are included, with excitation to levels above the Lorentz limit considered essentially as ionizing collisions. Recombination processes are negligible. The excited-level concentrations are shown in Table I for the three beam components typical of the ASDEX experiments. They amount to only about 0.5% for the $n=2$ level and decrease monotonically for higher levels.

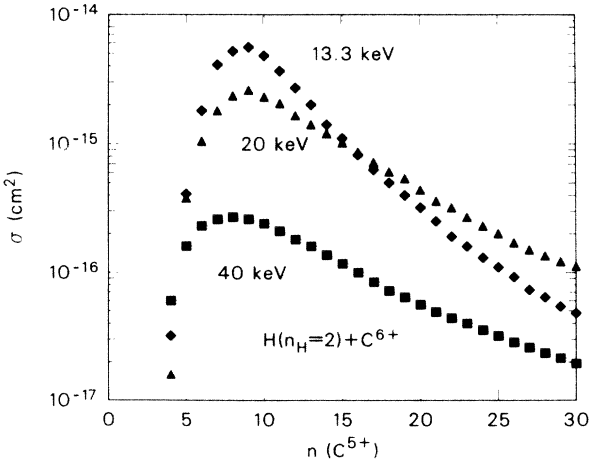

FIG. 3. Charge-transfer cross sections from hydrogen in the $n=2$ level to C^{6+}.

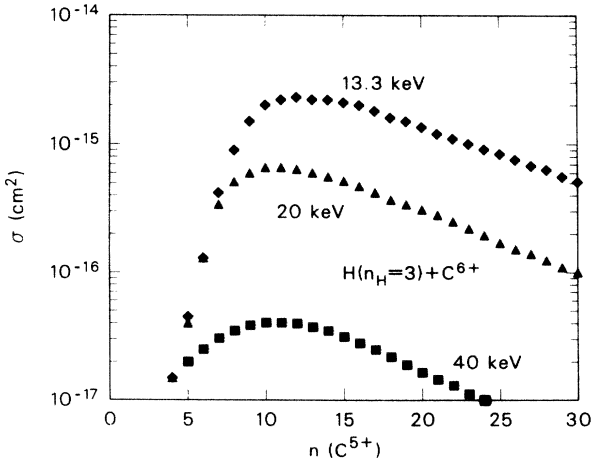

FIG. 4. Charge-transfer cross sections from hydrogen in the $n=3$ level to C^{6+}.

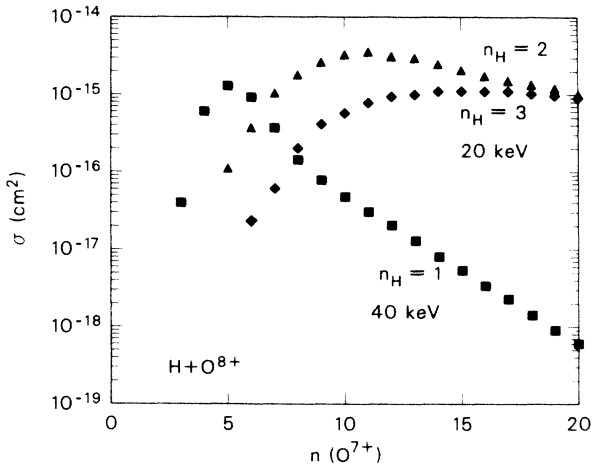

FIG. 5. Comparison of charge-exchange cross sections from the $n_H = 1,2,3$ levels of atomic hydrogen to excited levels of O^{7+}.

The influence of the excited states on the transitions of O^{7+} and C^{5+} has been investigated assuming equal currents in the three energy components of the neutral beams. Charge-transfer cross sections from the ground level for the 20.0- and 13.3-keV components, which are below the range of applicability of the classical trajectory Monte Carlo (CTMC) method, have been taken from Refs. 12 and 13; the data are extended up to $n = 20$ by assuming a straight-line extrapolation on a semilogarithmic scale.[13] It is not possible to include reactions with thermal ions; their velocities are below the range where the CTMC method is applicable, and cross sections for exciting individual levels have not been calculated by other methods, although the total capture rates have been estimated.[14] The weighted emission cross sections are computed by taking levels with $n = 7$ and above to be completely mixed for carbon ions and levels with $n = 8$ and above to be fully mixed for oxygen ions. Lower levels, characterized by the total angular momentum j rather than by the orbital angular momentum l, are assumed to be unmixed. Since all calculations of charge transfer treat l as a good quantum number, appropriate weighting of the cross sections is required to obtain the population rates for j states. In cases where only the total cross section for a given n level is available, statistical excitation of the angular momentum states is taken as a reasonable approximation.

TABLE I. Percent of total beam atoms in excited n levels for $T_e = 1000$ eV and $n_e = 5 \times 10^{13}$ cm^{-3}.

	E_{beam} (keV)		
n	40	20	13
2	0.62	0.49	0.39
3	0.27	0.24	0.21
4	0.10	0.10	0.09
5	0.05	0.04	0.04
6	0.03	0.02	0.02
7	0.02	0.01	0.01

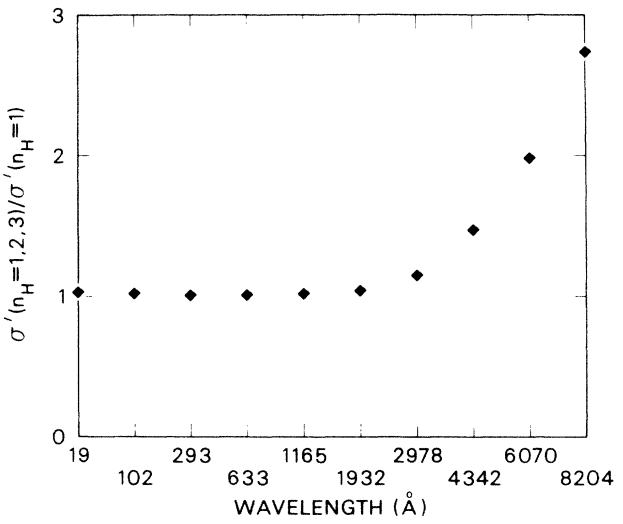

FIG. 6. Ratio of effective emission cross sections for O^{7+}. The values of σ' including excited hydrogen components are compared to those expected if only the ground state is populated. Excited hydrogen concentrations are taken from Table I, and the beam currents at 13.3, 20.0, and 40.0 keV are assumed equal.

Emission cross sections including and neglecting the excited hydrogen populations are compared in Figs. 6 and 7 for the $\Delta n = 1$ transitions. The excited states have little influence on the emission at short wavelengths, but above 2978 Å in oxygen and 3335 Å in carbon, their contribution to the emission cross sections becomes comparable to the contribution from the ground state. The increment of emission resulting from charge transfer out of

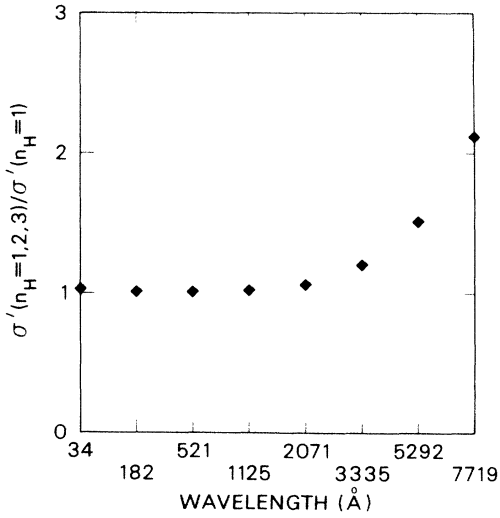

FIG. 7. Ratio of effective emission cross sections for C^{5+}. The values of σ' including excited hydrogen components are compared to those expected if only the ground state is populated. Excited hydrogen concentrations are taken from Table I, and the beam currents at 13.3, 20.0, and 40.0 keV are assumed equal.

the $n_H = 3$ level is only about 20% of the increment from the $n_H = 2$ level so it appears that higher excited states can be neglected. Clearly, though, the $n_H = 2$ and 3 levels must be taken into account if the beam in the field of view has significant fractions of low-energy components.

Although the present study was motivated by a desire to understand visible line intensities, it is of interest to examine the impact of excited hydrogen on x-ray emissions since the first experimental indications of an influence were obtained from the $nP \rightarrow 1S$ transitions of A^{16+}. Figure 8(a) indicates the relative intensities of the Lyman series of O^{7+} (except for Ly-α). Excited beam atoms have little influence on the stronger lines. The fact that Ly-δ is as strong as Ly-γ is a consequence of the fact that $n = 5$ is the level dominantly populated by charge transfer. The transitions from $n = 6$ and 7 are progressively weaker, but an increase of signal is apparent in the line from $n = 8$. This phenomena occurs because the present model treats all levels below $n = 8$ as unmixed but all higher levels as completely mixed. As a result, much of the population of the high angular momentum states is transferred into the shorter lived $j = \frac{1}{2}$ and $\frac{3}{2}$ states which can decay directly to the ground state. Figures 8(b) and 8(c) illustrate the relative intensities from levels having $n = 8$ and higher where the excited hydrogen does have an influence. It is seen that the signals are predicted to decay monotonically towards the series limit when the excited levels are not taken into account but that the decay is not so rapid when the populations of $n_H = 2$ and 3 are included in the simulation. In fact, the part of the series from the highest levels calculated appears as a narrow, flat continuum. In contrast, this pseudocontinuum actually rises to a peak around $n = 27$ in the experimental A^{16+} spectrum.[5] The difference possibly results from the fact that the thermal charge transfer occurs at $v_c/v_e < 1$ where the n_H^4 scaling holds, whereas at neutral beam energies, states higher than $n_H = 2$ do not strongly affect the emission.

In summary, we have shown that charge transfer from excited hydrogen can enhance the emission of visible and x-ray CXE lines from high-n levels of carbon and oxygen if significant currents of 10–20-keV atoms are present in neutral beams. If higher energy atoms dominate the beam composition, enhancements are small (e.g., a pure 40-keV beam or a nominal 120-keV beam for which the one-half- and one-third-energy components are 40 keV or greater). It must be emphasized, however, that the present analysis cannot account for additional contributions from low-energy thermal atoms which may have a current equal to 20% or more of the beam current and larger charge-transfer cross sections than the beam atoms. These particles are always present, so even when the beam purity or beam energy is high, enhancement from excited hydrogen is expected.

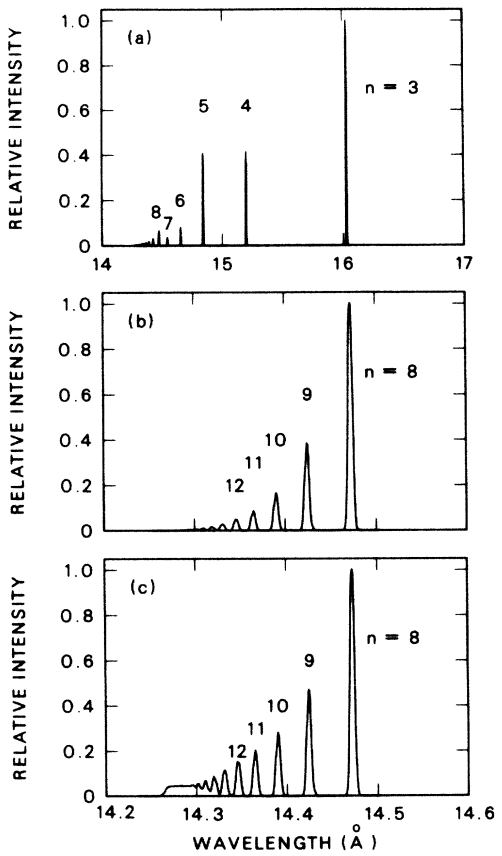

FIG. 8. Simulation of the Lyman series of O^{7+}: (a) $n = 3$ to $n = 30$, (b) $n = 8$ to $n = 30$ excluding contributions from excited hydrogen, (c) $n = 8$ to $n = 30$ including contributions from excited hydrogen.

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