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APRIL 1981

PPPL-1758

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IN TOKAMAKS: MOLECULAR ORIGIN AND
OBSERVATIONAL EFFECTS

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NARROW H-ALPHA EMISSION PROFILES IN TOKAMAKS:
MOLECULAR ORIGIN AND OBSERVATIONAL EFFECTS

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Abstract

The narrow hydrogen Balmer alpha profiles observed in tokamaks are explained in terms of the slow ($\sim 0.3\text{eV}$) and fast ($2\text{--}6\text{ eV}$) excited atoms formed by dissociation of molecular hydrogen at the plasma edge. Extra widening of the spectrum in the wings can be explained by Zeeman split H-alpha that is reflected from the vacuum vessel. This interpretation is consistent with available high-resolution data. The use of H-alpha as a diagnostic is discussed briefly.

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The narrow hydrogen Balmer alpha profiles (within 2 Å of the line center) from large tokamaks are usually attributed to atoms that have been slowed down by reflection from the walls and to excited 2-6 eV Franck-Condon atoms produced by electron reactions with H_2 molecules and H_2^+ ions. The "wall-reflected" neutral atoms are often assumed to have energies of ~ 20 eV based on the apparent Doppler width of the H_α (D_α) emission from these discharges. This interpretation involves two major difficulties. The first is the approximate invariance of the H_α linewidth for a wide variety of plasma parameters and wall conditions. The second is the high atom density derived from the apparent intensity of H_α emission by these 20 eV atoms compared to the density derived from neutral atom flux measurements at >30 eV. The invariance of the H_α linewidth suggests a molecular origin and dissociation is accepted as the origin of a 2-6 eV component when it is isolated in high resolution measurements; however, reactions involving H_2 or H_2^+ can yield few atoms with energies above 12 eV. In a tokamak the Zeeman shift of the H_α line in the large toroidal magnetic field can cause broadening far beyond the ~ 1 Å full-width-half-maximum that is characteristic of dissociatively excited H_α . A polarizer cannot completely eliminate the Zeeman shifted component if the wall viewed by the optical system reflects light from the plasma volume. The Zeeman effect must therefore be taken into account in order to correctly interpret the linewidth and intensity of the H_α line.

In this paper D_α spectral profiles are calculated under the assumption that the Balmer alpha emission originates in electron-impact reactions of D_2 and D_2^+ at the edge of a tokamak plasma. These reactions are first shown to produce atoms with energies of ~ 0.3 and $2-6$ eV. When Zeeman splitting and the reflection of light by the vacuum vessel are included, the calculated D_α profiles are in good agreement with high resolution spectra from the TFR tokamak. The significance of this molecular interpretation for the use of H_α light as a diagnostic in tokamaks is discussed briefly.

Origin of H_α . The kinetic energy distributions of the H atoms and H^+ ions formed in some electron-impact dissociation reactions of H_2 have been measured by time of flight^{1,2} and optical³ methods. When atoms (or ions) with these energies are observed in a plasma they can provide evidence of the presence of H_2 molecules in the discharge in the same sense that certain multiline spectra are "signatures" of H atoms or H_2 molecules. For example, excited product atoms in the $n=2-6$ states from the reaction $e+H_2+H^*+H+e$ (dissociative excitation of H_2)^{1,3} and, at high electron energies, apparently from the reaction $e+H_2+H+H^++2e$ (dissociative ionization of H_2) occur in two groups with characteristic energies of approximately 0.3 eV and $2-6$ eV. (We shall refer to these two groups as the slow and fast dissociation products, respectively.) Essentially the same energies are observed in the dissociative excitation of deuterium.¹ Product ions from the dissociative ionization of H_2 have been found experimentally² to have energies of roughly $2-12$ eV and the ions from the reaction $e+H_2^++H^++H+e$ (dissociative excitation of H_2^+) have been calculated to have energies in the same range,⁴ i.e., extending to slightly higher energies than the fast atom group formed in the dissociative excitation

of H_2 . (The ion energy measurements did not extend below 1 eV.) Numerous other processes involving H_2 and H_2^+ can produce atoms (possibly excited) and protons with kinetic energies in these ranges. The lack of accurate data on the kinetic energy distributions and, especially, on the excitation rates for many molecular processes makes it difficult to interpret quantitatively the atomic hydrogen line emission from plasmas which contain significant amounts of molecules.

The H_α profiles obtained by bombarding H_2 gas with an electron beam have a component of width $\lesssim 0.3 \text{ \AA}$ and a wider, flat-topped component of width $\sim 1 \text{ \AA}$ which correspond to the slow and fast dissociation products, respectively.³ H_α spectra whose structure is a result of the dissociative excitation of H_2 and other molecular reactions have been observed in low density ($n_e \sim 10^{12} \text{ cm}^{-3}$) plasmas.⁵ The plasma line shapes were somewhat different from those observed during electron beam bombardment of H_2 (for example, the characteristic "dissociation plateau" in the fast component spectrum is washed out) because of the isotropy of the plasmas and because of collisional heating of H_2^+ ions before they undergo such reactions as dissociative recombination ($e+H_2^+ \rightarrow H^*+H$) and dissociative excitation to yield H_α photons. Furthermore, under certain conditions, atoms with energies close to the dissociation energies (that is, atoms that were formed in dissociative reactions but have undergone few collisions) may be excited by electrons ($e+H \rightarrow H^*+e$) to yield H_α that is more or less indistinguishable from that produced by dissociative excitation.

In a large tokamak, of course, any molecular process must occur at the edge of the plasma since the mean free path for destruction of room temperature H_2 in a typical plasma ($n_e = 10^{13} \text{ cm}^{-3}$, $T_e = T_i = 100 \text{ eV}$) is roughly 3.5

mm. Similarly, few product atoms from H_2 (H_2^+) can reach the center as their mean free path is less than 5 cm. Highly energetic atoms can be formed at the limiter by neutralization of ions,⁶ and dissociation product atoms can, in effect, acquire high energies by successive charge exchange reactions and diffusion to the center of the plasma. Here we shall not be concerned with the Doppler broadened H_α spectrum of these "hot" atoms, which shows up as a wide, low-level background and whose structure is related to the spatial variation of plasma parameters such as T_i , n_H , and n_1 .

Zeeman effect and reflection of light. At the edge of a tokamak plasma, only the Zeeman shift will broaden the H_α produced by electron impact on H_2 (H_2^+) significantly beyond the ~ 0.3 Å and ~ 1 Å Doppler widths corresponding to the slow and fast dissociation products.⁷ At magnetic fields above 5 kG the Paschen-Back limit is applicable, so H_α will be split in accordance with the classical Zeeman effect.⁸ The total H_α emission over all solid angles in a high magnetic field is divided into three equally intense components: a central unshifted component and components shifted in wavelength by $-\Delta\lambda$ and $+\Delta\lambda$ relative to the unshifted H_α wavelength, where $\Delta\lambda$ (Å) = $0.02B$ (kG). Figure 1(a) illustrates the classical Zeeman effect in two special cases with a spectrum analyzer viewing a plasma perpendicular to a magnetic field (transverse Zeeman effect) and along the field (longitudinal Zeeman effect) with no reflections at the vessel walls. For observations perpendicular to the magnetic field B , if a polarizer is placed in the viewing path so that its polarization direction is parallel to the field, then the analyzer sees only the horizontally polarized, unshifted (π) component; if the polarizer is oriented perpendicular to the field, the analyzer sees two equal, vertically polarized, shifted components (σ) each with half the intensity of the π

component. If no polarizer is used, all three components are seen. Viewing along the field yields two equally intense, circularly polarized, shifted components.

Light reflected from the walls can form a significant portion of the observed light from a discharge in a toroidal vacuum vessel. Experience with Thomson scattering shows that the background plasma light level is often 20-40% higher when the viewing dump is removed. An experiment⁹ with different types of surfaces as viewing targets in the Elmo Bumpy Torus showed that reflected light made up at least 30% of the observed H_β signal when a smooth metal surface was seen by the detector. Returning to H_α , in a tokamak some of the H_α light reflected by the wall opposite a viewing port may come from near the optical axis (1B) of the viewing system [e.g., point T in Figure 1(b)] and will have a spectrum close to the transverse Zeeman effect. (If depolarization occurs during reflection, then a polarizer oriented parallel to the field will not completely eliminate the shifted components.) Reflected light coming from positions at large toroidal angles away from the viewing port [point L in Figure 1(b)] will be split in rough accordance with the longitudinal Zeeman effect and the split components cannot be removed by a polarizer. The Zeeman pattern for intermediate positions lies between these two extremes and multiple reflections may occur; thus, it is difficult to calculate the spectrum of the reflected light. It is clear, however, that reflected H_α light will normally contain a horizontally polarized shifted component unless special precautions are taken.

Calculation of D_α spectra in a tokamak. The preceding discussion can now be used for constructing the expected D_α spectrum from a tokamak. We consider

as an example a machine with a central toroidal magnetic field $B=40$ kG, a vacuum vessel major radius $R=80$ cm, and a discharge minor radius $a=20$ cm (the parameters of the TFR tokamak at the Centre d'Etudes Nucléaires, Fontenay-aux-Roses, France¹⁰). The energies of H and D formed in molecular reactions are at least approximately equal; therefore, based on the measured energies of product H atoms from H_2 and on the somewhat higher energies of H^+ ions from H_2 and H_2^+ , we assume for now that the fast dissociation product D atoms have kinetic energies of 2-10 eV and that the flat-topped (out to ± 0.3 Å) D_α fast component has a fwhm of 1.1 Å.¹¹ The D_α slow component has a fwhm of about 0.25 Å, including fine structure. In studies of electron-impact dissociative excitation of H_2 , the intensities of the fast and slow dissociative H_α components are found to be roughly equal for incident electron energies above about 35 eV,^{1,3} while the dissociation product ions from H_2^+ appear to belong mainly to the fast group.⁴ Since H_2^+ (rather than H_2) will be responsible for most of the H atoms at the edge of these plasmas, we shall assume that the intensity of the fast component is 3 times that of the slow (see reference 11). In the following examples we consider an optical system that views the plasma at 90° to the toroidal magnetic field through a port on the outside wall of the vacuum vessel in the toroidal midplane [cf. Figure 1(b)].

Figure 2(a) shows the D_α line shape when there are no reflections and a π polarizer (i.e., with its polarization direction parallel to the magnetic field) is used. This spectrum is equivalent to that with no polarizer in the absence of a magnetic field. The dashed horizontal line illustrates the decomposition of this profile into the flat-topped fast component ($\Delta\lambda_{1/2} \approx 1.1$ Å) and the weaker and narrower slow component (1/3 intensity and $\Delta\lambda_{1/2} \approx 0.25$ Å). If an instrument with a resolution of 0.5 Å were used to observe this

spectrum, the two components would be merged. If this profile (with a fwhm of $\sim 0.7 \text{ \AA}$) were then incorrectly assumed to correspond to a thermal distribution, the apparent "Doppler temperature" would be roughly 4 eV [$\Delta\lambda_{1/2}(\text{\AA}) = 0.36T^{1/2}(\text{eV})$]. Note that neither the fast nor the slow dissociation products have a Maxwellian energy distribution.^{1,5}

Figure 2(b) shows the D_α profile for a 40 kG magnetic field with no reflections and no polarizer. The dashed curves represent the three Zeeman components (a central component and two equal shifted ones with half its intensity), while the solid curve shows the combined profile. If this curve is smoothed to simulate an instrument resolution of about 0.5 $\text{\AA}$, the result is a profile with a fwhm of 1.5 $\text{\AA}$, for an apparent Doppler temperature of the D atoms of about 18 eV. A polarizer is customarily used to eliminate the Zeeman shifted components under the assumption that there are no reflections from the wall opposite the viewing port. When this assumption is valid, the spectrum seen through a π polarizer is that of Figure 2(a).

The profile that results when 30% of the total observed D_α intensity is randomly reflected light and a π polarizer is used is shown in Figure 2(c). Here "random" means that one third of the reflected light is centered at each of $\Delta\lambda = 0.8, 0$, and $-0.8 \text{ \AA}$ (low level dashed curves). The combined spectrum is denoted by the solid curve. No instrument broadening or smearing of the shifted components owing to the radial variation of the magnetic field is included. This profile is the same as that which would be obtained if 20% of the total signal were light which had been reflected into the collecting optics from positions at large distances from the viewing port [i.e., all the reflected light were Zeeman split; cf. point L of Figure 1(b)]. Here, despite the use of a polarizer, the spectrum extends out to 1.5 $\text{\AA}$ on both sides.

When 50% of the total D_{α} signal is randomly reflected light and a π polarizer is used, the spectrum has the form shown in Figure 2(d). This spectrum is the same as if one third of the total signal were reflected light originating far from the viewing port, perhaps because of the orientation of the surface seen by the spectrum analyzer. As before, the contributions of the unreflected signal and of the reflected components are shown in the form of dashed curves and the total signal is a solid curve. The dot-dashed curve extending beyond $+0.7 \text{ \AA}$ illustrates the smearing of the Zeeman split components in the radially varying magnetic field. (Here it is assumed that equal amounts of reflected light come from all radii inside the torus.) Again, the spectrum extends to at least $1.5 \text{ \AA}$ on either side.

Comparison with published data. Fabry-Perot interferometers have been used to observe the time history of the replacement of deuterium by hydrogen (and vice versa) within a single discharge and over series of discharges in the ATC¹² and DITE¹³ tokamaks. The H_{α} and D_{α} linewidths observed in these experiments were less than $1 \text{ \AA}$ and suggest that the emitting H atoms may have the molecular dissociation energies [cf. the discussion of Figure 2(a) in the preceding section]. The spectral resolution, however, was not sufficient to allow separation of the fast and slow dissociation components and the free spectral range was too low to provide any information on the wings of the profile. Thus, from the standpoint of spectral structure or atom energies, these data only imply that the "average" energy is about 2-3 eV and that the profiles have enhanced wings.

The best reported high-resolution H_{α} and D_{α} spectral data have been taken on the TFR tokamak.^{10,14} Figure 2(e) (solid curve) shows a D_{α} spectrum from a

discharge in D_2 with $B=40kG$ taken with a Fabry-Perot interferometer at a resolution of $0.1 \text{ \AA}$ and viewed at 80° with respect to the toroidal magnetic field through a π polarizer.¹⁴ (The published spectra are quite reproducible but not symmetric; only half of one trace is shown here. No further details were provided on the observation conditions.) The smeared profile of Figure 2(d) is also shown in Figure 2(e) (circles) for comparison. The model calculation clearly exhibits the major features of the experimental profile: a narrow peak which is resolved into two components together with a wing that is relatively flat out to about $1 \text{ \AA}$ and falls off by about $1.5 \text{ \AA}$. The viewing direction in the experiment is so close to 90° that the relative error in our calculation for 90° is negligible in comparison with the intensity of the apparent reflected light. The earlier fall-off in the wings of the observed profile may be caused by a smaller contribution to the reflected light from the inside of the torus (higher field region) than from the outside. However, this earlier fall-off is most likely related to the narrower width of the observed profile in the $0.25\text{-}0.6 \text{ \AA}$ interval, which corresponds to the unreflected fast dissociation product component. If it is assumed (see reference 11) that the fast dissociation product atoms from D_2^+ have energies of $2\text{-}6 \text{ eV}$ (that is, the same energies as those from D_2), rather than $2\text{-}10 \text{ eV}$, then the fast component width is reduced to approximately $0.8 \text{ \AA}$ from $1.1 \text{ \AA}$ and the calculated and observed spectra are in almost complete agreement. The ratio of the areas of the fast and slow components is then 2.2. The TFR data therefore suggest that the kinetic energy spectrum of the product atoms from D_2 and D_2^+ are similar and that the same dissociating molecular states are probably responsible for excited atom formation in both cases.

The flat top of the fast dissociation product component shows up clearly in the TFR data as a shoulder at $\Delta\lambda \sim 0.3 \text{ \AA}$. As mentioned previously, this shoulder was not seen in some colder plasmas. In the tokamak the H_2^+ ions formed as a result of ionization of H_2 will move along the magnetic field and most of the velocity gained by them in Coulomb collisions will be along the field lines (i.e., isotropy will not be established before dissociation occurs); thus, the velocity of H_2^+ perpendicular to the field lines should differ little from that of the cold H_2 from which it was formed. The H_α spectrum from the tokamak is therefore closer to that from electron beam experiments³ than are the spectra from certain low density plasmas.⁵

A lower resolution ($0.3 \text{ \AA}$) D_α spectrum from TFR under similar conditions is shown in Figure 2(f) (solid curve).^{10,14} The curve of Figure 2(d) with smoothing to account for an instrument resolution of $0.3 \text{ \AA}$ is also shown (circles) for comparison. Here the spectrum seems to have only two components, a narrow and a broad one, with apparent widths corresponding to "Doppler temperatures" for "Gaussian" profiles of about 1 eV and 30 eV, respectively. The agreement between the model and the observations is good, particularly if the above modification is made in the energy spectrum of the fast dissociation products. It is clear, however, that a nonthermal distribution is actually responsible for both the theoretical profile and, as can be seen in the higher resolution data of Figure 2(e), the experimental.

Conclusion and discussion. The D_α data from TFR can be fitted fairly accurately by assuming that the narrow ($\Delta\lambda < 1 \text{ \AA}$) profile comes from atoms produced in molecular dissociation reactions involving D_2 and D_2^+ and that the broad profile is caused by a reflected Zeeman component that cannot be

eliminated by a polarizer. The presence in the narrow D_α profile of components from both the slow and fast dissociation product groups is evidence of the presence of molecular hydrogen at the edge of the discharge. The high resolution data also suggest that the kinetic energy distribution of excited $D(H)$ atoms from D_2^+ (which are more numerous than those from D_2 in the plasma boundary layer if $T_e \gtrsim 10-15$ eV) is close to that of the atoms formed from D_2 . Specific details of the spectrum in the wings (the "broad" component) will obviously depend on the magnetic field strength, the optical reflection characteristics of the wall seen by the analyzer optics, the properties of the plasma in the source volume, and the radial distance between the vacuum vessel wall and the limiter. Thus, for certain operating conditions or machine designs, the wings may be much smaller or entirely absent. It is essential that a good viewing dump be used in any experiment from which spectral profile or intensity information is to be obtained. Conversely, the presence of the wings may provide information on the amount of reflected light in optical signals from the plasma. This analysis does not exclude the possibility of a small contribution (above the wide background spectrum from the "hot" atoms in the plasma) from a population of atoms with energies on the order of 30 eV, but this appears inconsistent with the peculiar shape of the broad component in the high resolution data.

It seems appropriate to conclude by examining the consequences of this analysis for plasma diagnostics in tokamaks using hydrogen line emission. Because of its inevitable presence in hydrogen discharges, hydrogen line emission is an obvious and potentially informative diagnostic. It is not, however, a simple task to extract quantitative information from it. Perhaps smaller devices whose edges are more easily studied can be used to develop

this diagnostic technique. The interpretation of the narrow H_α emission profiles given here clearly implies that molecular processes are important at the plasma edge. The kinetic energy distribution of the "cold" H atoms (formed by molecular dissociation) observed in high resolution spectra is physically distinct from that of the "hot" atoms in the main plasma (formed by recombination and, effectively, by charge exchange). Consequently, the H_α intensity and linewidth data are not necessarily in conflict with data⁶ from neutral atom flux analyzers--the relation between the two may be complex, involving many intermediate steps. It is tempting to regard the H_α emission from a plasma as a direct indicator of its particle confinement properties.¹⁵ H_α data may be suitable for this purpose if the spectra from the "hot" and the "cold" atoms can be distinguished. High resolution, along with complete elimination of the Zeeman split components, is required to separate them. The narrow molecular H_α line profile can be simply related to the gross particle confinement time for the entire discharge only if molecules, from gas feed and wall recycling, are the sole source of atoms entering the plasma. The narrow peaks in the H_2 -D₂ replacement studies¹³ appear to be caused by molecular dissociation. Their intensity is thus related to a kind of recycling rate for molecules rather than atoms, although the basic conclusions of reference 13 are still valid because the molecules do produce atoms which enter the plasma. In general, other sources of atoms, such as limiter interactions and neutral beam injection, which may be more significant to the discharge, must be included in the particle balance. The most serious limitation on a quantitative analysis of H_α is the lack of adequate cross-section data for H_α excitation in various reactions involving H_2 and H_2^+ . The re-excitation of fresh dissociation product atoms, the kinetic energies and relative populations of atoms in different states, and the

modification of molecular cross sections owing to vibrational excitation must also be taken into account in order to determine, from observations of H_{α} light, the flux of molecules and atoms entering a discharge.

ACKNOWLEDGEMENTS

I would like to thank Jim Cobble (O.R.N.L.) and Ernesto Mazzucato for showing me their data. This work was supported by the U.S. Department of Energy, Contract Number DE-AC02-76-CH0-3073.

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spectrum will be somewhat smaller. This appears to be the case according to the spectral data that are discussed later in this paper.

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FIGURE CAPTIONS

Figure 1. (a) Illustrating the transverse and longitudinal Zeeman effects.
(b) A top view of a segment of the toroidal midplane of a tokamak showing an optical viewing port and reflected light reaching it from positions close to (T) and far from (L) it. (809068).

Figure 2. (a)-(d) Calculated D_{α} spectral profiles in a 40 kG magnetic field for various reflection conditions and polarizers. Spectral profiles from the TFR tokamak (solid curves) for 0.1Å (e) and 0.3Å (f) resolution compared with theoretical profiles (circles). (809069).

(a) ZEEMAN EFFECT

(b) REFLECTIONS IN A TORUS

Fig. 1. (PPPL-80906B)

Fig. 2. (PPPL-809069)