Plasma diagnostics with spectral profile calculations

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A method is presented to interpret spectroscopic measurements to obtain a diagnostic of conditions in hot, dense plasmas using a fast computer code to calculate the theoretical profiles of the ionic spectra emitted. The method employed involves the computation of the spectral shape of the ionic transitions with the plasma electron temperature and density as parameters, a convolution of this theoretical profile with the instrument function, and a comparison of the resulting profile with the experimental spectrum. The computation is performed using an atomic physics data set coupled to a fast version of a line shape code that is capable of considering an extremely large number of sublevels for each transition. The plasma electron density and temperature are the only free parameters and the complex shape of the calculated line profile serves as a signature of the plasma conditions. Published spectral measurements of several ionic transitions of Li-like C and N in a hydrogen plasma are considered as an example. For certain of these transitions, the possibility of the observation of an ion dynamics effect on the ionic emitters is discussed.

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I. INTRODUCTION

The interpretation of experimental measurements of spectra emitted by complex ions in hot, dense plasmas is often limited by the fact that the spectral line profiles which contain the information required for a diagnostic of the plasma conditions are rarely composed of simple combinations of known shapes such as Lorentzian or Voigt. This means that usually the entire profile of the radiation emitted in the spectral region of the transition under study must be computed and compared with the measurements in order to permit a determination of the plasma temperature and density. For hot and dense plasmas where the principal emitters can be highly ionized species, a complicated calculation involving complex atomic physics coupled with line shape theory is required. In the following it is shown that the use of a fast computer code, developed for the computation of these ionic transition profiles under very general plasma conditions [1], can be used as a new and powerful tool for plasma diagnostics.

The computation of the spectral shape of ionic lines emitted from plasmas requires an intricate combination of the electron collision operator for the various Stark components, the Stark effect of the ion microfield at the radiator, and the slow fluctuation of this microfield (if necessary). The atomic physics data for these complex ions must also be obtained. This means that the calculation of the spectral shapes of these complex ionic transitions is much more involved than the isolated or independent linewidth computations that are often used to obtain the electron density of a weakly ionized, low temperature plasma. With highly ionized atoms, the ion Stark effect, in general, can act on a large number of levels belonging to the set of upper or lower states involved in the transition and the profile calculation that must be carried out can involve hundreds of sublevels. This often results in a complicated spectral profile which has a behavior with varying plasma conditions that cannot be described by a simple functional dependence on the electron density. This, of course, is well known and has been discussed thoroughly in the literature [2]. The fast computer code of Ref. [1], developed particularly for the computation of the spectra emitted from hot dense plasmas, is capable of dealing with the large arrays required for the transitions in these highly excited ions. A description of the capacity for calculation of this code will be given in Sec. II.

In the past, due to the lack of an efficient method for obtaining theoretical profiles to aid in the interpretation of spectral data, approximate scaling formulas have been suggested which fit the variation in half width to a function of the electron density. However, even slight differences in the experimental conditions from those used in the theory can result in errors in the analysis. A good example of these problems can be found in the use of the scaling formulas of Ref. [3] to analyze data for the spectra from highly excited states of several carbon and nitrogen ions [4] that was taken under experimental conditions different from that for which the relations were designed. Difficulties in interpretation exist also for the transitions from lower excited states of the Li-like C and

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N ions [5,6] as will be seen in the following.

The conclusion to be drawn from the results of the code analysis, presented in the ensuing sections, is that no simple scaling function can yield as useful a general diagnostic as a complete calculation of the spectral profile. The half width of the line, for example, is sensitive to the plasma electron density even though the line shape is not a simple combination of Lorentz, Voigt, or Stark shapes. The dependence of the profile on the plasma conditions is complicated, however, because it arises from the separate contributions of the Stark components of the radiative transition, each of which has an average position, width, and intensity that varies with electron density and temperature. In addition, the amplitude, shift, and the presence or absence of fine structure and plasma induced forbidden components also contribute to the shape of the overall spectral profile. Each particular transition, therefore, will have a shape with a specific dependence on the electron density that serves as a signature of the plasma conditions from which the line was emitted. It is this particular dependence on the environment of the radiating ion which enables the spectral profile to be used for diagnostic information. The fact that essentially no simple formula can describe the profile dependence on electron density and temperature means that a complete profile calculation is required to use spectral line shapes as a diagnostic of hot, dense plasmas. The ability of this code to compute complete line shapes is, therefore, a powerful instrument for plasma diagnostics. Finally, it is to be emphasized that the only parameters in the calculations are the plasma density and temperature and that because of the complexity of the profiles, a simple superposition of the profiles often suffices for a diagnostic.

For the comparison of the theoretical computation with an experimental spectrum, the calculated profile must also be convolved with Doppler broadening (if necessary) and the apparatus response function. These convolutions are especially important for the diagnostic of the plasma, especially in cases where the associated widths are comparable to the plasma broadening. This is because the inverse process, the deconvolution of the experimental profile to obtain the underlying line shape, cannot be performed uniquely. That is, given an experimental profile obtained with an instrument with an apparatus function comparable to the linewidth, the profile that would have been observed with a perfect instrument cannot be uniquely obtained by deconvolution. On the other hand, a calculation of the profile of the considered transition has a shape with a characteristic dependence on the plasma conditions and when convolved with the slit function provides a spectrum which can be compared with data.

Using line shapes for plasma diagnostics, therefore depends critically on the underlying calculation of the spectral profile. This is particularly apparent in the example considered in Sec. III where the experimental observations of a series of high resolution spectra from excited state transitions of Li-like ions of carbon and nitrogen in a hydrogen plasma [5] are discussed. These particular spectral transitions are interesting because of their importance in vacuum ultraviolet (vuv) recombination laser development where the laser gain is sensitive to the embedded line width of the particular profile component that arises from an inverted transition [7]. They also are of interest for the analysis of the radiation emitted in recent experiments on inertial confinement plasmas [8] and in astrophysical calculations of the carbon abundance as well as in radiation transport in stellar interiors [9]. The original interpretation of the spectral profiles observed in the experiment of Ref. [5] was extremely difficult in the absence of a complete calculation of the line shape because of the large apparatus function. The computation presented here, however, enables a much better understanding of these measurements. For example, it is shown that the measured profiles of all the spectra are consistent with emission from a homogeneous plasma at an electron density and temperature different from that originally published with the spectral data. In addition, the computed line profiles suggest different identifications of certain spectral features in the published data. This will be considered in greater detail in the discussion of the experimental investigation presented in Sec. III. There the use of the code calculations is shown to offer a dramatic improvement in the use of spectral profiles for plasma diagnostics.

The analysis of the spectra of Ref. [5] will also contain a discussion of the possibility of observing some of the first evidence of an ion dynamic effect involving highly charged radiators. In the past, this effect has been proposed as a possible mechanism affecting the spectroscopic interpretation of the radiation from plasmas [10]. Some indication of the presence of ion dynamics also appears in Ref. [6]. For certain of the lines studied in Refs. [5] and [6], ion dynamics will be found to be an important effect on the theoretical profile. However, the large apparatus function present in the experimental data, when convolved with the theoretical profile means that the observation of the effect becomes marginal. Nevertheless, it is important to note that, in general, if ion dynamics were to be neglected, the raw spectral data might yield a profile which would be interpreted as if produced by plasma conditions different from those actually present in the experiment. Thus there is a need to perform a complete calculation of the spectral profile, including the ion microfield fluctuations, before comparing the theoretical line shape to the experimental profile for the diagnostic of the plasma conditions in the general case.

II. CALCULATIONS

The calculational method used to obtain the shape of the spectrum emitted by a plasma is based on the usual separation of the effects on the radiating ion of the fast electron impact collisions and the slowly moving ion quasistatic Stark field. This approximation considers the perturbing ion microfield at the radiator to act first and split each radiative transition into a number of Stark components. The electron collisions then become a relaxation mechanism for these components in the same manner as, and in addition to, the spontaneous emission. These electron collisions, therefore, result in the homogeneous broadening of each Stark component of the radiative transition. As a first assumption, the perturbing ions are considered to be static during the radiation process and an average over the microfield perturbation at the radiator is performed to obtain the inhomogeneous broadening contribution to the line shape. In the approximation used for the calculation at this stage, a fixed number of statistically distributed microfield values for each radiative transition are used to calculate the line shape. This produces a profile that can be described by the sum of a finite number of components for each radiative transition. These components are characterized by a central frequency, a homogeneous width, and a complex amplitude [1]. At this stage, the approximate code calculation can be thought of as modeling the profile of each radiative transition by a weighted sum of the radiation arising from a finite number of separate channels (the radiative components). These separate radiative channels contribute to the final spectral profile according to their amplitude or probability of occurrence.

This picture is correct, however, only if the ion microfield does not change during the radiation process. If the ion microfield fluctuates, the radiation will be transferred from channel to channel within each radiative transition during this time and the line profile will become a complex mixture of the radiative components of the static calculation. To account for this transfer of excitation in the calculation, a particular model is postulated. The radiative channels belonging to each transition are assumed to be mixed together at a given frequency determined by the ion microfield fluctuation rate. In this manner, the ion dynamic is simulated in the code by the dynamical mixing of the field averaged radiative components, obtained from the static calculation for each radiative transition separately. The idea behind this model is the assumption that the component mixing is the result of sudden microfield fluctuations at the radiator. In this it is analogous to the collisional line mixing effect studied in atomic and molecular spectroscopy [11]. The rate of component mixing in this model is taken to be the inverse of the decorrelation time of the plasma microfield and can be calculated from a simulation of the electric field fluctuations in the plasma or, for highly charged ions, from a simple model of plasma fluctuations.

In the calculation, the dynamical mixing produces an additional broadening and shift of each component. The different radiative transitions are not mixed together in this model; only the radiative components of each transition are combined. Because of this, in the limit of a very large fluctuation or mixing rate, the components collapse back into the original line associated with the radiative transition and the sole effect of the plasma on the profile is the homogeneous electron broadening. This means that when the ion microfield fluctuates rapidly, the line shape is dominated by impact collisions, as expected. This limit of the Stark component mixing is analogous to the narrowing of Doppler broadened transitions in the presence of a large velocity changing collision frequency. In the opposite limit, a small mixing rate, the quasistatic limit is recovered as is required. Similar to the collisional line mixing studies cited in Ref. [11], these calculations show that the ion dynamics effect can result in an important modification of the overall transition profile in some cases.

The number of radiative components which must be mixed to simulate the effect of ion dynamics is quite large in general. For the example to be discussed in this article, the $\Delta n = 1$ transitions of C IV and N V, the levels involved have the typical doublet structure characteristic of Li-like ions. Here each transition will have, in the absence of the ion microfield, three radiative constituents corresponding to $|\Delta J| = 0, 1$. When immersed in the plasma, these three transitions are shifted and split by the plasma Stark effect which divides each radiative transition into a large number of radiative channels. The number of these channels will be equal to the product of the number of upper and lower sublevels considered for each state of the ion microfield that occurs. To obtain the total number of channels which must be considered, this quantity is multiplied by the number of microfield states used in the microfield average. (In practice, the number used for the computation is much less than this total due to the occurrence of zero amplitude or equal frequency components which, of course, are not mixed.) It can be seen, however, that the analysis of the half width of the transition requires a large computation and can only be performed by taking into account many more radiative channels than the three original transitions. A simple analysis based only on fitting a Lorentzian or static profile to the three unperturbed radiative transitions would not be useful for plasma diagnostics. An accurate calculation must be performed if a comparison between the theoretical and experimental line shape is to be utilized for diagnostic purposes. As will be seen in Sec. III, this is even more important when a large apparatus function is present in the observed profile.

To illustrate the ion dynamics effect on the theoretical line profile, the result of the code calculation for the C IV $4d$-$3p$ transition in a plasma with electron density $N_e = 2.2 \times 10^{18}$ cm^{-3} and temperature $T_e = 10.7$ eV is displayed in Fig. 1(a). The plasma conditions, used in this figure, have been chosen because they produce profiles which match the experimental data that are to be analyzed in Sec. III. The spectral shape is presented in the figure with and without ion dynamics in the calculation. The forbidden $4f$-$3p$ line can be seen in the short wavelength wing of the static profile of the resonance transition. The ion dynamic effect results in the mixing and resultant merging of this feature into a single asymmetric resonance so that the line shape with ion dynamics included has only an asymmetry on the short wavelength side of the line rather than the separate forbidden resonance line seen in the static profile.

A similar effect can be seen in Fig. 1(b) where the same $4d$-$3p$ transition in N V is calculated for identical plasma conditions. In the static microfield calculation for this ion, the fine structure components can be seen to be well separated in the central region while the forbidden, $4f$-$3p$, components are seen in the line wing. The calculation including ion dynamics results in the merging of the fine structure and the forbidden transitions with the main line and, as in the previous case, results in an asymmetric but smooth profile.

Similar calculations have been performed on the $4f$-$3d$

and the $n=5$ to 4 transitions of C IV and N V with results that are comparable to those discussed above. In Sec. III, the spectral shape of all of these transitions will be compared to the experimental spectra of Ref. [5]. As noted in the Introduction, for this purpose the calculated profiles are convolved with the instrument function. For the large apparatus function in these data, this convolution produces a profile in which much of the detail and asymmetries seen in the spectral shape generated by the computation are partially smoothed. The loss of information that is associated with the convolution always occurs, of course, when the apparatus profile has a width comparable to that of the spectral profile being analyzed. The smoothing due to the apparatus function is in addition to that resulting from the ion dynamics and these two effects should not be confused. In any case, it should be clear that simple methods of analysis which suggest that the data be fit either with the three Lorentzians corresponding to the fine structure transitions or with the quasistatic line shape alone will not give an accurate diagnostic of the plasma. In circumstances such as those studied here, the experimental data can only be used for an accurate diagnostic of the plasma conditions through the detailed calculation of the profile which contains the information that is lost in the convolution with the apparatus function.

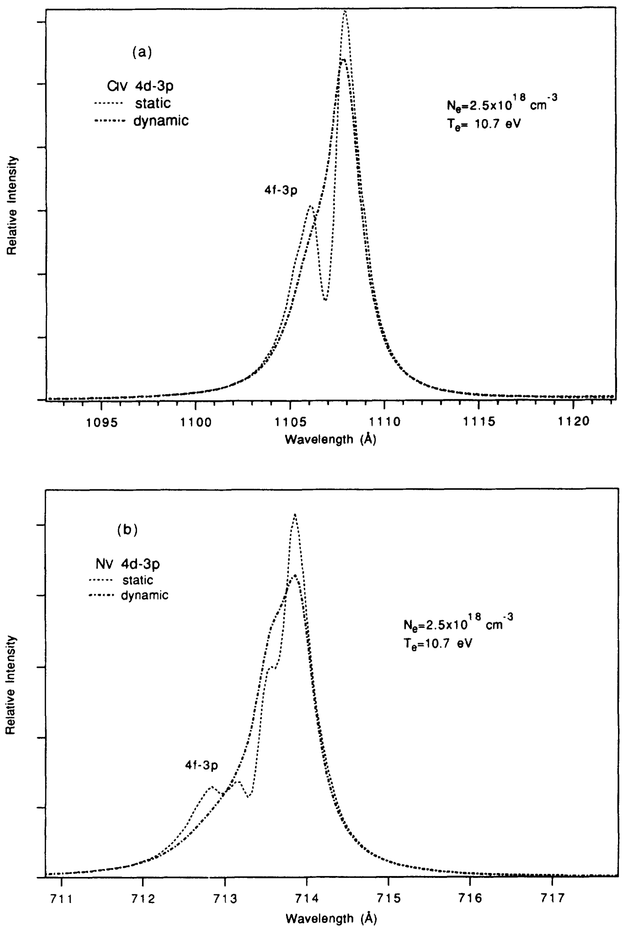


FIG. 1. (a) The theoretical line shapes of the lithiumlike carbon C IV dipole-allowed $4d$-$3p$ transition at 1108 Å and the associated dipole-forbidden $4f$-$3p$ transition at 1106 Å. The line profiles are presented as relative intensity versus wavelength in angstroms. The electron density N_e is 2.2×10^{18} cm^{-3} and the temperature T_e is 10.7 eV. The dot-dashed curve denotes the calculation including ion dynamic effects and the dashed curve that in which the microfield is static. Note that the forbidden transition which is a definite feature in the static theory merges into the resonance line when ion dynamics is included in the computation. (b) The theoretical line shape for the lithiumlike nitrogen N V, dipole-allowed $4d$-$3p$ transition at 713.8 Å and the associated dipole-forbidden $4f$-$3p$ transition at 713 Å. The fine structure components near line center and the forbidden lines on the high energy wing provide distinct features of the static profile (dashed curve) which are merged into an asymmetric line profile by the ion dynamics (dot-dashed curve).

III. PLASMA DIAGNOSTICS

The data to be examined in the following are taken from the measurements published in Ref. [5]. These experiments were performed with a gas-liner pinch that permitted accurate spectral measurements of a test gas (the atomic species of interest) in a stable, homogeneous hydrogen plasma at high electron density and temperature. The hydrogen, which is the driver gas in the pinch, forms a hot and dense central plasma column in which varying amounts of the test gas are injected along the axis in the central region where it becomes concentrated with homogeneous plasma conditions. The procedure for obtaining the spectral data for the lines and a slightly different version of this experimental apparatus is described elsewhere [12]. The plasma temperature was determined from the C IV to C III line intensity ratio and checked with the blackbody limited intensity of an optically thick C IV resonance transition. The electron density was obtained from the width of the He II $P\alpha$ line using an empirical relationship [13], which was verified later using Thompson scattering [11]. The measurement of the plasma conditions in these experiments, therefore, carries a high degree of confidence. Several of the transitions of Ref. [5] were remeasured recently with essentially the same plasma apparatus, but with upgraded diagnostics to verify the line shapes [6]. In addition, measurements of the $n=3$ to 3 transitions of these and other Li-like ions have been performed [14], and verified with the improved diagnostics [15], again with similar temperatures and densities. Various $n=7$ to 6 ionic transitions have also been studied in the same manner [4].

The superposition of the calculated theoretical and the experimental spectral profiles measured in Ref. [5] imply an electron density which is a factor of 3 larger than that published with the data. The reason for this difference has not been determined, but a similar discrepancy has been noted in the value of the electron density given in similar measurements of the $n=3$ lines by the same group [14] and that found in their subsequent remeasurement of these lines [15]. These experiments measured lines with similar half widths, but apparently different plasma conditions and differ only in that improved diagnostics were used in the later experiment. The explanation given in Ref. [15] was that the neglect of even small amounts of the test-gas ions could lead to underestimates of the electron density by as much as a factor of 3. This discrepancy is the same as that found in the present study. In addition, the comparison of the data of Ref. [5] with the more recent measurements of the half width of some of these lines in Ref. [6] indicates that the higher density deduced here from the line shape analysis is consistent with the remeasured line widths.

The apparatus profile in first order is quoted in Ref. [5] as being a combination of a Voigt profile with a 0.01 nm Gaussian, full width at half maximum (FWHM), and a 0.17 nm Lorentzian, FWHM. Doppler broadening was negligible for all the spectra measured. The C IV $n=4$ to 3 transitions as well as the N V $n=5$ to 4 lines were measured with second order resolution. The narrower N V $n=4$ to 3 lines were measured in fourth order. In all of these cases, the instrument width is of the same order of magnitude or less than the plasma broadening, so that the convolution with our calculations and the comparison with the data can give an accurate diagnostic of the plasma parameters. The C IV $n=5$ to 4 transition was measured in first order and here the large apparatus function limits the accuracy of the comparison.

In Fig. 2(a), the effect of the convolution with the apparatus profile on the calculation of the $4d$-$3p$ transition of C IV is illustrated. The theoretical profile that was presented in Fig. 1(a) is here convolved with the instrument width and compared to the experimental data. For this comparison, the same electron density $N_e=2.2\times10^{18}$ cm^{-3} and temperature $T_e=10.7$ eV as that in the calculations shown in Fig. 1 was used. As expected, the structure due to the forbidden $4f$-$3p$ transition, washed out in the ion dynamic calculation, is now seen to be only a slight asymmetry of the line profile. The same profile calculated with a static environment and convolved with the apparatus function still retains a large knee at the $4f$-$3p$ line position. The absence of a separate forbidden line feature in the resultant profile, therefore, serves as a signature of the ion dynamics. The excellent agreement of the experimental points with the ion dynamic computation seen in Fig. 2(a) suggests that ion dynamics effects may be present in the data. A measurement with higher resolution would be desirable to confirm the existence of the ion dynamics effect. Finally, the position of the merged forbidden line depends on the electron density and affects the observed line asymmetry. The calculation produces the correct asymmetry only with the separation of this component from the $3p$-$4d$ C IV resonance line consistent with an electron density of 2×10^{18} cm^{-3}. This is further evidence for the correctness of the assumed plasma conditions.

The same $4d$-$3p$ transition in N V with identical plasma parameters is presented in Fig. 2(b). This figure depicts the convolution of the theoretical profile of Fig. 1(b) with the apparatus function in fourth order. Again the agreement between the theoretical profile and the experimental points is quite good; however, here the difference between the static and dynamic shapes is not as great as for C IV. Nevertheless, the absence of the asymmetry associated with the convolution of the static line shape again suggests the presence of ion dynamics effects on the profile.

The comparisons presented in these figures display the effect of the apparatus function convolution on the calculated theoretical profiles presented in Figs. 1(a) and 1(b). They also permit an identification of some of the features seen in the experimental profiles. This understanding is very important for a spectral region like that of the next transition to be considered, the C IV $4f$-$3d$ transition. Here the presence of C III transitions in the wing of the

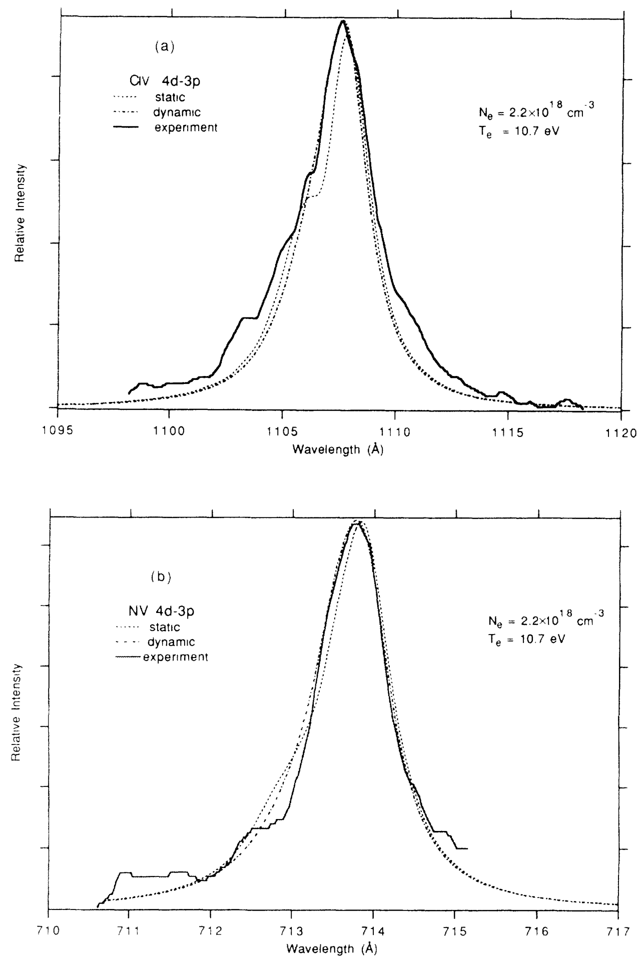


FIG. 2. (a) The theoretical C IV $4d$-$3p$ dipole-allowed transition profile compared to the experiment. The plasma conditions are the same as in Fig. 1, but the theoretical profiles have been convolved with the second order apparatus function (approximately 0.9 Å FWHM) for comparison with the experiment. The data points are indicated by the solid line and the two convolution calculations are labeled as in Fig. 1. The ion dynamic profile is seen to be in good agreement with the experiment. (b) The theoretical N V $4d$-$3p$ profiles compared to the experiment. The plasma conditions are the same as in Fig. 1, but the theoretical curves have been convolved with the fourth order apparatus function (approximately 0.45 Å FWHM) for comparison with the experiment. The data points are indicated by the solid line and the calculation is labeled as in Fig. 1. Note the good agreement of the theory with the ion dynamics profile.

profile could lead to a large uncertainty in obtaining the spectral line shape. For example, a resonance in the long wavelength wing of the experimental profile of this line, originally identified in Ref. [5] as the forbidden $4d$-$3d$ transition, can be shown to arise from a line associated with C III transitions which occur at this wavelength. The $4d$-$3d$ forbidden line is not observed in the wing because it is merged with the allowed transition by the ion dynamics. This is illustrated in Fig. 3(a), which displays the theoretical line profile of the C IV $4f$-$3d$ line before the convolution with the apparatus function. The forbidden line in the long wavelength wing of the static calculation can be seen to merge into the resonance line when ion dynamics are included.

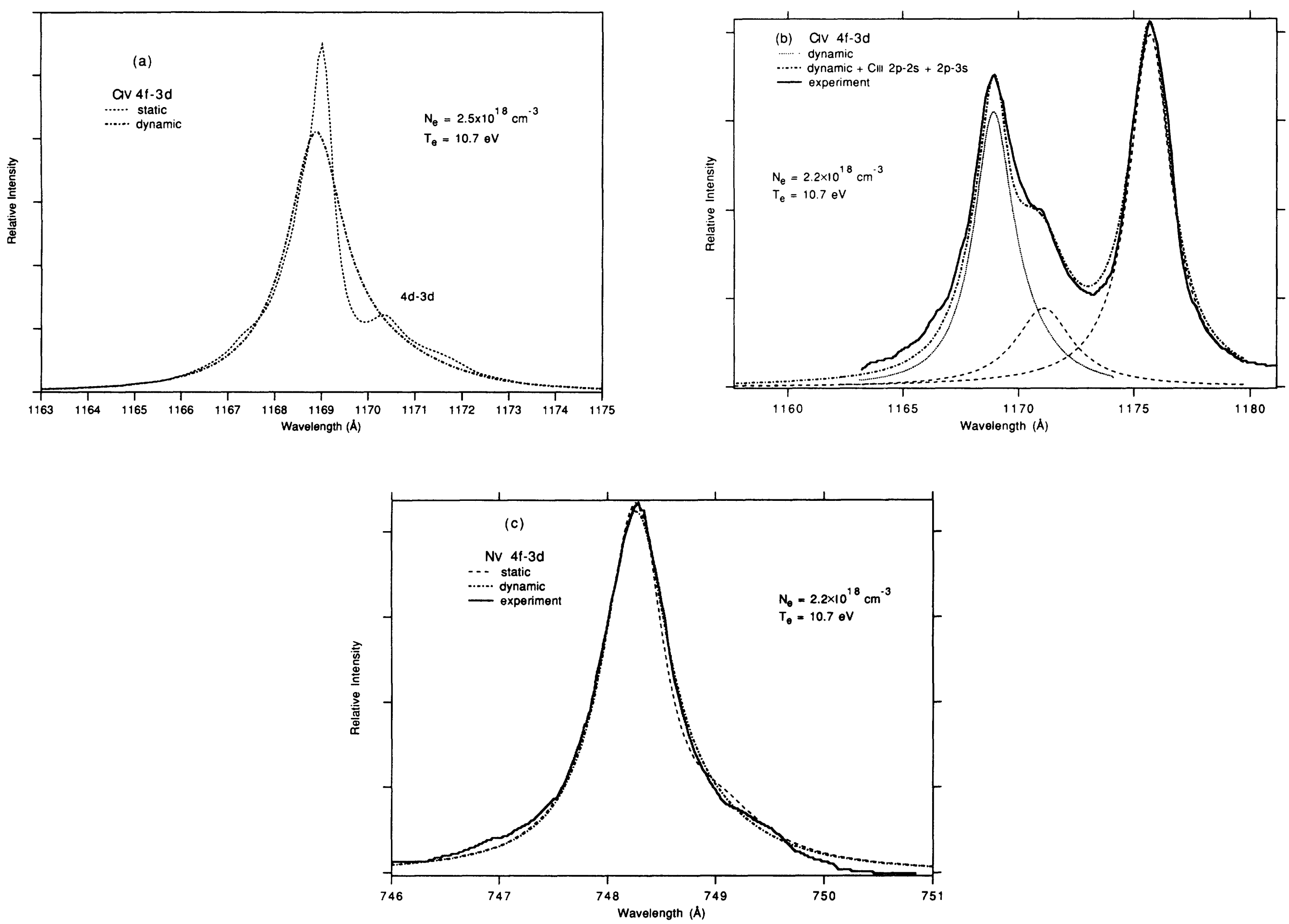
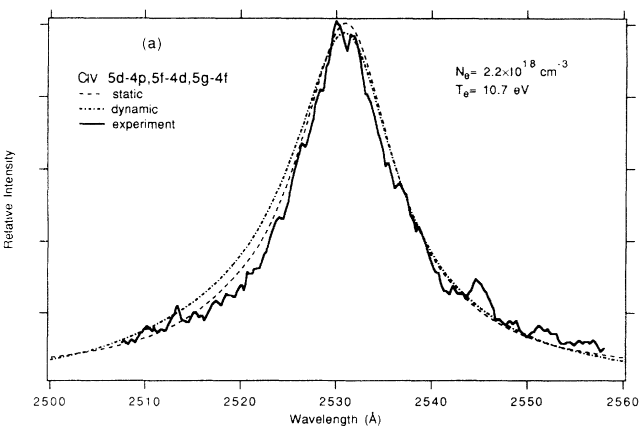


FIG. 3. (a) The theoretical line shape for the lithiumlike carbon C IV, dipole-allowed $4f$-$3d$ transition at 1169 Å and the associated dipole-forbidden $4d$-$3d$ transition at 1171.5 Å. The line profiles are displayed as relative intensity versus wavelength in angstroms and the dot-dashed curve is the theory with ion dynamics effects while the dashed curve is the static microfield calculation. The plasma conditions are the same as for the preceding figures, with electron density $N_e = 2.2\times10^{18}$ cm^{-3} and temperature $T_e = 10.7$ eV. The merging and complete disappearance of the forbidden transition when ion dynamics is taken into account is an important feature of this profile. (b) The comparison of the theoretical C IV $4f$-$3d$ profile to the experiment. The plasma conditions are the same as in (a), but the theoretical curves have been convolved with the second order apparatus function (approximately 0.9 Å FWHM) for comparison with the experimental data. The experimental points are indicated by the solid line and the calculations are labeled as in (a). Included also is the contribution of the C III $2p^2$-$2p2s$ line at 1176 Å in second order and the 585 Å C III $2p3s$-$2p^2$ line at 1171 Å in fourth order, individually treated as Lorentzian contributions and shown as dashed lines. The total of the theory including ion dynamics and these two lines is represented by the dot-dashed line. This total line shape can be seen to be in good agreement with the data points. (c) The comparison of the theory and experiment for the N V $4f$-$3d$ transition at 748.2 Å. The theory includes a convolution with the apparatus profile (approximately 0.45 Å FWHM) for the fourth order dispersion. The line profile is presented as relative intensity versus wavelength in angstroms, the data points are indicated by the solid line, the dot-dashed curve is the theory with ion dynamics effects while the dashed curve is the static microfield calculation. The plasma conditions are the same as in the preceding figures. Good agreement with the theory including ion dynamics can be seen.

In Fig. 3(b) the experimental spectrum of the C IV $4f$-$3d$ line measured in second order is compared to the convolution of the theoretical profile of Fig. 3(a) with the apparatus function. The data, again from Ref. [5], display both the C III $2p^2$-$2p2s$ line at 1176 Å and the 585 Å C III $2p3s$-$2p^2$ line (at 1171 Å in fourth order) in the red wing of the C IV $4f$-$3d$ transition. These C III lines were found also in the remeasurement of the C IV $4f$-$3d$ line published in Ref. [6]. When the two C III Lorentzians are added into the wing of the resonance line computation, good agreement is obtained with the observed spectral shape of this transition. This is seen in Fig. 3(b), where the data are compared with the spectrum obtained by the convolution with the apparatus function of the sum of the theoretical profile of Fig. 3(a) and the C III $2p^2$-$2p3s$ and C III $2p3s$-$2p^2$ Lorentz shaped lines. This calculation has been performed using the same plasma electron density and temperature as in the previous profile calculations.



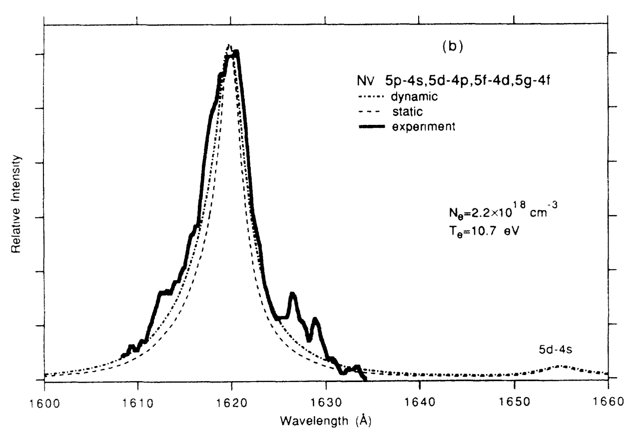


FIG. 4. (a) The overlapping $5p$-$4s$, $5d$-$4p$, $5f$-$4d$, and $5g$-$4f$ lines of C IV compared to the experimental data for the same plasma conditions as in the preceding figures. The data points are indicated by the solid line. The theory includes a convolution with the first order apparatus profile (approximately 1.8 Å FWHM) and the dot-dashed curve is the theory with ion dynamics effects while the dashed curve is the static microfield calculation. Only a small difference in the static and dynamic profiles exists. (b) The overlapping $5p$-$4s$, $5d$-$4p$, $5f$-$4d$, and $5g$-$4f$ lines of N V compared to the experimental data for the same plasma conditions as in the preceding figures. The data points are indicated by the solid line. The theory includes a convolution with the first order apparatus profile (approximately 1.8 Å FWHM) and the dot-dashed curve is the theory with ion dynamics effects while the dashed curve is the static microfield calculation. Only a small difference in the static and dynamic profiles can be seen.

The shape of the corresponding $4f$-$3d$ transition in N V, which is unaffected by nearby resonances, has been calculated using identical plasma conditions. The convolution with the fourth order apparatus function is given in Fig. 3(c) and is seen to match closely the experimental profile. In both Figs. 3(b) and 3(c) there is a slight difference in the half widths calculated with and without ion dynamics, but this effect can be seen to be less important than for the transitions considered above and is probably unobservable except with data of extremely high resolution.

The other transitions measured in this set of experiments were the overlapping $5p$-$4s$, $5d$-$4p$, $5f$-$4d$, and $5g$-$4f$ lines of both C IV and N V. Here again, because of the complications arising from the large number of radiative transitions and the even larger number of associated Stark components, it is crucial to have a good computational model of the line profile in order to perform diagnostics with the observed line shape. Figures 4(a) and 4(b) display the line profiles for these transitions in C IV and N V, respectively, as calculated with the same electron density and temperature as in the previous comparisons, but this time the convolution is performed with the much larger first order apparatus function. The difference between the static and dynamic profiles is very small, and the accord with the experimental data is slightly worse than for the other transitions. Nevertheless, the consistency of the agreement at the same temperature and density for all of these transitions provides strong evidence of the reproducibility of the experiment and the validity of the line shape modeling.

IV. CONCLUSION

A computer code, developed for the calculation of the spectral profile of lines emitted by a complex ion in a plasma, has been shown to be a powerful tool for the diagnostic of the plasma parameters. In particular, the theoretical calculation of the line shapes enables the use of spectroscopic measurements for the determination of the plasma conditions. The profiles of a set of Li-like vuv transitions of carbon and nitrogen have been calculated and compared to experimental data as an example of the method. The computed and measured profiles are in excellent agreement and are consistent with the same electron temperature and density. It is to be noted that in spite of an instrumental profile in these experiments which was of the same order as the plasma broadening, the accurate calculation of the line shape permitted a good diagnostic of the physical conditions of the plasma. This analysis would not have been feasible without the calculation of the complete line profile. In addition, as is illustrated in the analysis of the C IV $4f$-$3d$ line, the identification of spectral features as either forbidden lines or impurity lines superimposed on the transition is only possible with a complete line shape calculation.

Some indication of an ion dynamics effect has also been presented. This effect, which has been observed to strongly affect some lines emitted by neutral atoms in plasmas, has not previously been definitively identified in radiation from ionized emitters in a plasma. The finding here, that the effect should exist for some of the considered transitions and is absent for others, means that in the analysis of the experimental profiles of lines emitted by ions in hot dense plasmas, one must be extremely careful to consider this effect when using the line shape as a diagnostic. On the other hand, the variation of the ion dynamics effects with transition can provide further information on the plasma conditions, since a set of line shapes could exhibit a characteristic behavior with respect to plasma temperature and density.

More generally, the importance of the results presented here lies in the major extension of the diagnostic value of spectral line shapes for plasma studies. The agreement with the experimental observations provides substantive proof of this assertion. In the past the utility of plasma line shape diagnostics was limited by two factors: first, a complete theoretical model, including some major effects, e.g., ion dynamics, did not exist; and second, a rapid line shape computational method that could handle transitions of arbitrary complexity within the theoretical model was not available. These limitations led to a severe restriction on the use of spectral line shapes as a diagnostic tool. Experimentally the observation of simple transition types, i.e., those from K-shell emitters or isolated lines, were the only reliable source of information, but, as we have shown here, previous attempts to analyze even the simpler Li-like spectra were restricted by the lack of a sufficient model [3–5]. Moreover, the usual limitations imposed by the experimental constraints such as the availability of instruments with sufficient resolution or the requirement of particular plasma conditions, etc., often obviated the use of spectral line shapes as a diagnostic. We emphasize that the computational model, used above, largely removes these constraints. For this reason, the accurate modeling of spectral line shapes arising from transitions in complex ions in hot, dense plasmas and the analysis of the associated experimental data is now possible.

In conclusion, the ability to calculate line shapes from arbitrary transitions, including all the dominant effects, is now available with the code described here. In addition, ions far more complex than those used to illustrate this article could be considered, thereby providing an avenue by which to attack large complex problems for diagnostic purposes. It is to be noted that the current capability of the code has been applied to level structures with as many as one thousand states.

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