Stark broadening of resonance transitions in B III

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We performed line profile measurements of the $2s$-$2p$ resonance transitions in B III in order to test quantum-mechanical (close-coupling) theory. The experiment was carried out using the well-diagnosed gas-liner pinch discharge where plasma parameters are determined independently by 90° Thomson scattering. The experimental Stark widths are about twice the five-state close-coupling results. However, we find good agreement with semiclassical calculations in the electron-impact approximation.

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I. INTRODUCTION

When calculating opacities of large-scale plasmas, e.g., of stellar atmospheres, the Stark-broadened line profiles of resonance transitions are of the utmost importance because they give a relatively large contribution to radiative energy transport [1,2]. In this respect the simplest atomic systems are lithiumlike ions where the corresponding energy levels are nondegenerate and only one electron is outside of the first closed shell. In most situations their resonance lines will be well isolated and electron-impact broadening will dominate the linewidth. Therefore, their line profiles provide an excellent test of the theoretical approximations, in particular we will compare our experimental results with recently performed quantum-mechanical calculations using close-coupling theory [3].

On the one hand, since the upper levels $2p\ ^2P^o_{3/2}$ and $2p\ ^2P^o_{1/2}$ of the resonance lines are predominantly perturbed by their lower level $2s\ ^2S_{1/2}$, the calculation would seem to be possible with a small but sufficient set of states leading to high accuracy. This advantage for theoretical calculations, on the other hand, gives rise to experimental difficulties, namely, only relatively small Stark broadening will occur when compared with spectral lines from more highly excited levels. For this reason there are only two experiments on the Stark broadening of $2s$-$2p$ transitions in lithiumlike Be II [4,5]. The comparison with close-coupling calculations by Refs. [3,4] shows that the experimental data of both experiments are larger than the theoretical results by a factor of about 2. Although these experiments suggest errors in the close-coupling calculations the experimental data were not accurate or convincing enough to motivate theoretical studies.

In addition, there are a number of experiments on resonance transitions of more complicated ions, e.g., of Ca II and Mg II (see compilations of experimental and theoretical data in Refs. [6]). However, most of these data are not of the required accuracy to test available close-coupling calculations. Furthermore, the experimental results obtained by different groups differ by a factor of about 2. The situation is even worse since some of the more advanced experiments [7] obtained results that show increasing Stark widths with increasing electron temperature. This finding is in contradiction to many experiments on electron-impact-broadened line profiles performed by different experimental groups [8–11] and to theoretical calculations [12–16].

Therefore, an accurate experiment is vital to test close-coupling calculations. This is particulary apparent as the close-coupling calculations of Sanchez *et al.* [4] and Seaton [3], which both include exchange, differ by a factor of about 1.4 for low temperatures. At present, this discrepancy between the two close-coupling calculations [3,4] is not understood.

In order to test the calculations we performed measurements of the line profiles of the $2s\ ^2S_{1/2}$–$2p\ ^2P^o_{3/2}$ and $2s\ ^2S_{1/2}$–$2p\ ^2P^o_{1/2}$ resonance transitions in B III in the well-diagnosed plasma produced by a gas-liner pinch discharge. The experimental results are compared with semiempirical [15], semiclassical [1,17], and with close-coupling calculations [3].

II. EXPERIMENT

The gas-liner pinch resembles a large-aspect-ratio z pinch characterized by two independent fast gas inlet systems [18,19]. Boron is introduced by means of the first electromagnetic valve using very small amounts of borontrifluoride (the so-called test gas). It is injected along the axis of the discharge chamber through a nozzle in the center of the upper cathode. The second electromagnetic valve injects hydrogen (the so-called driver gas) through an annular nozzle of 17-cm diameter in the upper electrode. Initially, the driver gas forms a hollow gas cylinder near the wall. The gas is dissociated and preionized by discharging a 50-nF capacitor (20 kV) through 50 needles which are mounted underneath the lower cathode on an annulus. Finally, the discharge of a 11.1-μF capacitor (27 kV) through the initial preionized gas shell results in a compression of the gas cylinder to a plasma column of 1–2 cm in diameter and 5 cm length. The compression time is 3 μs and the lifetime of the plasma is about 0.5 μs.

The proper choice of the time of injection and of the amount of the test gas ensures that the test gas ions are located in the central homogeneous part of the plasma column. For relatively small test gas concentrations as used in this study the radial and axial homogeneity of the plasma column

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is verified in Refs. [8,9,11]. In Ref. [8] we demonstrated the radial homogeneity by measuring continuum and line radiation from test gas ions from a single discharge transversely resolved to the plasma axis. An Abel inversion of the measured intensities showed that the test gas ions are distributed in the central homogeneous part of the plasma. In Ref. [9] we verified this result with Thomson scattering, and in Ref. [11] the axial homogeneity of the plasma is demonstrated measuring line radiation from test gas ions from a single discharge spatially resolved along the plasma axis. Therefore, there is no cold boundary layer for the emitting (test gas) ions, and, in general, optically thin plasma conditions can be produced for almost all spectral lines. The reproducibility of the plasma is directly measured with Thomson scattering [20] (see below). Furthermore, we detect the discharge current with a Rogowski coil and the plasma radiation at 520 nm with a $\frac{1}{4}$-m monochromator which is equipped with a RCA 1P28 photomultiplier. This signal is also used to measure the time delay between the maximum pinch compression and the detector settings.

Spectroscopic line profile measurements and Thomson scattering are performed side-on using a 1-m spectrometer (Spex model 1704) in the visible spectral range. The slit height and width are chosen to be 2 mm and 50 μm, respectively. The spectral line profiles are detected in sixth order with an optical multichannel analyzer (OMA, EG&G model 1456B-990G) using a 1,200 lines/mm grating blazed at 750 nm and an interference filter (Schott, UV-KMD) in order to suppress radiation from other orders. This mounting is nescessary to achieve a sufficiently high resolution of 0.0025 nm/pixel. It gives for the plasma parameters of the present study an apparatus and Doppler width which together do not exceed 33% of the total measured linewidths full-width at half maximum (FWHM). By recording hydrogen continuum radiation without injection of test gas we ensure that the detection system (including the interference filter) has equal sensitivity over the small wavelength range of the $2s\ ^2S_{1/2}$–$2p\ ^2P^o_{3/2}$ and $2s\ ^2S_{1/2}$–$2p\ ^2P^o_{1/2}$ resonance lines of B III. These measurements also confirm that there is no unwanted impurity radiation from residual gas in the discharge tube affecting the spectrum in the investigated wavelength interval. The wavelength calibration of the detection system over a wavelength interval of $180<\lambda<280$ nm is carried out by employing Fe and Al hollow cathode lamps. Further, their spectra yield the apparatus profile which is properly taken into account in the data analysis (see below). Besides using hollow cathode or spectral lamps which are only useful for a measurement of the apparatus function in the cw mode of the detector, we also measured the apparatus profile in the pulsed mode with Rayleigh scattering on propane. This is accomplished over the full dynamic range of the detection system by properly varying the propane gas pressure. No differences between both methods could be found and the apparatus profile is given by a Voigt function with 0.0071-nm Lorentzian FWHM and 0.0049-nm Gaussian FWHM. For the present spectral line profile measurements the gating time of the OMA detector was 35 ns, i.e., about the same time as the duration of the ruby laser pulse which determines the time resolution of our diagnostic procedure.

We utilize 90° Thomson scattering to independently diagnose the plasma [22,23]. For this purpose we focused a ruby laser (2 J with a pulse width of 25–35-ns FWHM) into the center of the plasma column. For the present plasma parameters observing the scattered laser light at an angle of 90° gives a scattering parameter $\alpha>1$. For that reason only the ion feature of the scattering spectrum could be observed. The analysis of the ion feature of the Thomson scattering spectra gives the proton, electron, and test gas ion temperature when fitting the theoretical form factor of Ref. [24] to the experimental scattering data by a least-squares procedure. We find the same value for the ion, electron, and test gas ion temperature. Electron densities are determined by calibrating the detection system with Rayleigh scattering on propane and using the fitted (frequency-dependent) form factor to obtain the frequency-integrated form factor by numerical integration. For very small test gas (impurity) concentrations as used in this study there are no deviations of this procedure from conventional methods using the Salpeter approximation to determine the frequency-integrated form factor [23]. Estimating the mean charge number of the test gas ions from spectroscopic measurements allows us to determine the test gas ion concentration from the relative intensity of the so-called impurity peak of the scattering spectrum. In this way the concentration of boron ions is estimated to be less than 0.3% of the electron density in all cases. As shown below this concentration gives optically thin plasma conditions for the investigated spectral lines.

III. RESULTS AND DISCUSSION

We found a suitable plasma condition for line-shape measurements shortly after maximum pinch compression. For about 50 ns the plasma parameters did not change appreciably, and at this time during the discharge the test gas ions are distributed in the central homogeneous part of the plasma column. The mean values of the measured plasma parameters along with the rms values obtained from ten measurements are shown in Table I. We carried out nine spectroscopic measurements at this condition and fitted two independent Voigt functions (one for each multiplet component) to the experimental data by a least-squares procedure. Figure 1 shows an example of a measured spectrum along with the fitted Voigt function. The Voigt functions consist of the measured apparatus profile, a Doppler profile calculated according to the measured ion temperature, and a Lorentzian with variable width to determine the Stark broadening. For each spectrum both multiplet components give the same width (FWHM) for the Lorentzians to within 5%. The fits also indicate that the line profiles are not distorted by any other spectral line from B III. Even the relatively strong $4f$-$3d$ transitions at $\lambda=207.71$ nm is of negligible intensity. The $4f$-$3d$ line is observed only when increasing the test gas concentration by more than a factor of 10. The mean values of the fitted Lorentzians, i.e., the Stark widths of the measured spectra are also given in Table I. Their rms values are 12% and 11% for the $\frac{1}{2}$-$\frac{1}{2}$ and $\frac{1}{2}$-$\frac{3}{2}$ component, respectively, indicating the good reproducibility of the measurements. In Table I we added an additional error of 2% to these values. This is done to take into account the uncertainty in the determination of the measured temperature and hence of the Doppler contribution to the measured linewidth. Zeeman broadening is negligible at our plasma conditions [8]. The

TABLE I. Experimental Stark widths w_m (FWHM) of the investigated $2s$-$2p$ transitions in Li-like boron. Experimental results are compared with theoretical widths w_G calculated after Ref. [1], w_{DK} after Ref. [15], w_{HB} after Ref. [17], and w_S after Ref. [3]. The error of w_m includes an error estimate for the Doppler contribution to the measured linewidth.

Ion	Transition array	Multiplet (No.)	Wavelength (0.1 nm)	Temperature (10^4 K)	Electron density (10^{18} cm^{-3})	w_m (0.1 nm)	$\frac{w_m}{w_G}$	$\frac{w_m}{w_{DK}}$	$\frac{w_m}{w_{HB}}$	$\frac{w_m}{w_S}$
B III	$2s$-$2p$	^2S- $^2P°$	2067.33	10.6±17%	1.81±13%	0.220±14%	1.19	2.14	1.24	1.79
		(1)	2065.87	10.6±17%	1.81±13%	0.221±13%	1.19	2.15	1.24	1.81

fitting procedure also gives the relative intensities of both multiplet lines. They are found to be 2:1 for each spectrum with a deviation smaller than 4%. This value is in good agreement with the predictions of the LS-coupling approximation, i.e., 2.00:1 and confirm that the spectral lines are optically thin. Deviations from the prediction of the LS-coupling approximation to smaller values than 2 could be found only when increasing the amount of test gas in the discharge by a factor of 5.

In Table I we compare the experimental Stark widths (FWHM) with theoretical calculations for the measured plasma parameters after Refs. [1,3,15,17]. The semiempirical method of Dimitrijević and Konjević [15] extends expressions of the earlier investigation of Griem [25] and takes into account dipole-allowed electron collisions. The Gaunt factor is chosen empirically according to Refs. [14,26] and its extrapolation to below threshold energies also accounts for elastic scattering [25]. The semiclassical approximation of Griem [Eq. (526) of Ref. [1]] is slightly modified according to the author's suggestions introducing effective principle quantum numbers and Bates-Damgaard factors. The latter were taken from Refs. [27,28]. Besides dipole-allowed electron collisions an estimate of the strong collision term is also included which accounts for about 12% of the total calculated width. Griem gives further a rough estimate of the ion quadrupole broadening. Although according to Ref. [1] this contribution may be about 10% of the total calculated width it is not included in the calculations because it is too roughly known. For example, recent detailed calculations of the ion quadrupole broadening of the $3s$-$3p$ transitions of the Li-like ions C IV–Ne VIII show that this additional broadening contribution is smaller than 5% of the Stark width [29]. Dipole-allowed proton collisions are completely neglegible for the present experiment [1,16]. The use of the theoretical approximations of Hey and Breger [17] is extensively discussed in Refs. [8,21]. These authors chose different procedures from those of Griem [1] to calculate the minimum and maximum impact parameters of the electron collision process. Although their strong collision term is appreciably larger, even for the relatively low charge state of the studied ion, their resulting widths differ only slightly from that of Griem. The five-state close-coupling calculations shown in Table I are taken from Seaton [3]. The data are given for a set of electron temperatures and for the present plasma parameters, where the Stark broadening is less dependent on the temperature, the theoretical value is obtained by interpolation with an error smaller than 1%. In addition, we used a linear scaling in electron density to scale the theoretical broadening values to the density of the present experiment. This is justified because Debye shielding effects are not important for our plasma parameters.

Figure 2 shows the experimental data compared to the calculations for an electron density of $n_e = 1.81\times10^{18}$ cm^{-3}. The experimental error bar is 20% of the measured Stark width and takes into account the errors of the linewidth measurement, of the electron density determination, and of

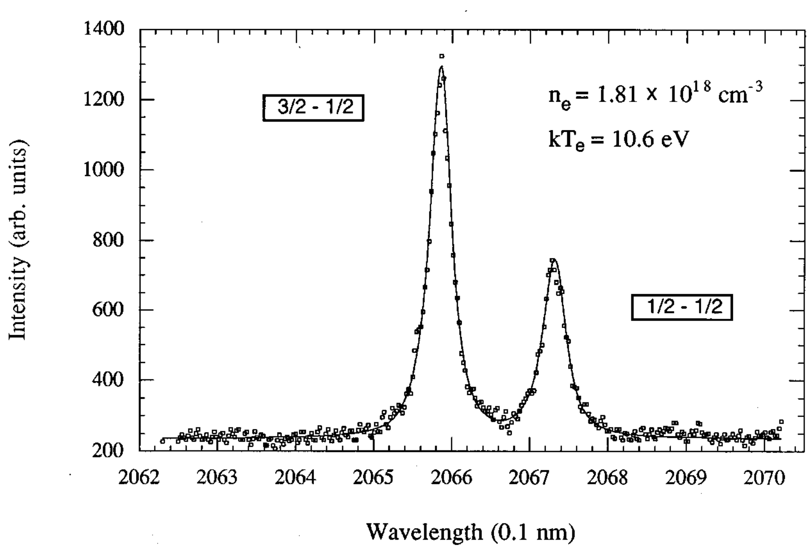

FIG. 1. Example of a recorded line spectrum; □, measured; —, Voigt function best fit. Electron density and temperature are obtained from Thomson scattering.

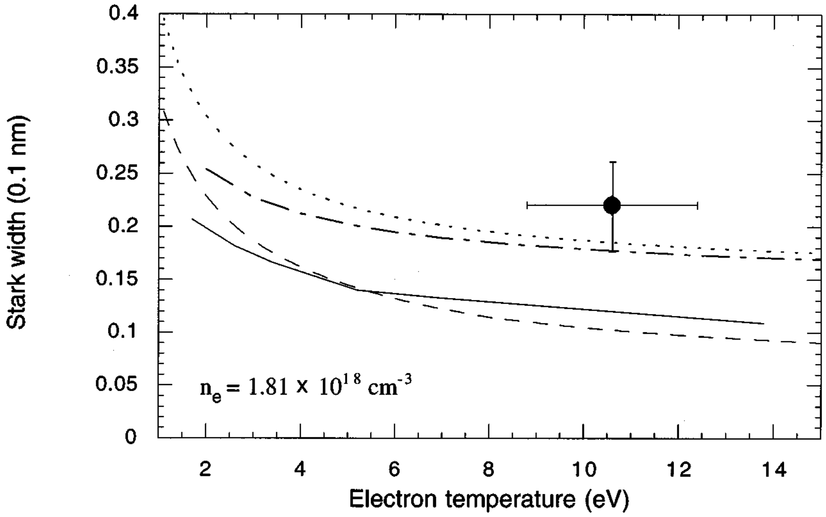

FIG. 2. Comparison of the experimental Stark width (FWHM) of the $2s$-$2p$ transitions in B III with the results of the theoretical approximations after Griem [1]: ····, after Dimitrijević and Konjević [15]: - - -, by Hey and Breger [17]: - · · · · -, and from Seaton: —. The electron density is $n_e = 1.81 \times 10^{18}$ cm^{-3}. The vertical error bar takes into account the errors of the measured line profiles, of the convoluted Doppler profile, and of the electron density determination.

the Doppler contribution to the linewidth. It becomes obvious that the semiclassical calculations are in good agreement with the experimental Stark widths. The remaining discrepancies of about 20% might partially be explained by ion quadrupole broadening. Since this contribution to the linewidth appears to be marginal, more detailed calculations are necessary to determine the importance of this additional term for the linewidths of electron-impact-broadened spectral lines. On the other hand, there is a surprisingly large difference between the measured Stark width and the calculated widths using the semiempirical approximation of Ref. [15] or the five-state close-coupling calculations of Ref. [3]. While the discrepancy with the semiempirical approximation may be due to the neglect of strong collisions there is no simple explanation for the failure of the values given in Ref. [3].

In an earlier investigation we found that both approximations predict systematically lower Stark widths for spectral lines of higher ionized species ($Z>3$, where Z is the spectroscopic charge number) than experimentally observed [8]. In these cases, however, the discrepancies with Seaton's close-coupling calculations are clearly due to the neglect of perturbing levels with principal quantum numbers $n>3$ in the calculations. Indeed, the agreement of measured Stark widths of the $3s$-$3p$ transitions in C IV [8] with quantum mechanical theory is improved when comparing with nine-state close-coupling calculations of Ref. [30]. For the $2s$-$2p$ transitions of the present study, however, a similar improvement by including more perturbing levels in the calculations is not expected since the corresponding collision rates are much smaller than in case of the $3s$-$3p$ transitions of C IV [31]. As also pointed out in Ref. [4] a possible explanation for the deviations of close-coupling calculations from the present experimental data and semiclassical calculations are large cancellations of direct and mixed terms in the expression for the linewidth. Hence, small errors in the calculations of the transition-matrix elements result in large errors in the linewidth. This assumption is further supported by the differences between close-coupling calculations of different authors as mentioned in the Introduction.

IV. CONCLUSIONS

We find that the experimental line profiles of the $2s$-$2p$ resonance transitions in B III are not in agreement with the most elaborate linewidth calculations based on quantum mechanical (close-coupling) theory. The discrepancy between the experimental and the theoretical Stark widths is almost a factor of 2. On the other hand, good agreement of the experimental profiles with several semiclassical calculations is obtained. Since the $2s$-$2p$ spectral lines of lithiumlike ions are the simplest transitions to calculate because they are nondegenerate, the present measurements provide a benchmark for electron-impact line-shape theories. In particular, it is important to understand the failure of the close-coupling calculations since *a priori* they should be the most accurate. Hence, with the advent of widely employed fast computers the use of close-coupling calculations for line shapes in a number of fields, e.g., plasma physics, astrophysics, or molecular physics, will burgeon. If a systematic problem renders the close-coupling calculations inaccurate it is essential that new theoretical studies be performed.

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