Stark broadening of germanium

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(Received 30 May 1974)

Stark broadening parameters of the more prominent visible germanium lines are measured in a 1-eV shock-tube plasma. Estimated accuracies for eight observed Ge II and two Ge I lines are (10–30)%. Ionic results are compared with semiclassical predictions. Agreement with theory is excellent for two of the three observed multiplets, but unaccountably poor for the third. Moreover, widths of the two lines in this third multiplet ($5s\ ^2S$–$5p\ ^2P$) are grossly different from one another. Possible sources for this anomaly are discussed.

I. INTRODUCTION

Measurements of Stark-broadening parameters provide means for diagnosing laboratory and astrophysical plasmas, for computing radiative transfer in extended atmospheres, and for testing theoretical descriptions of density-dependent emission.[1-4]

This work tests the reliability of a semiclassical model which embodies a simple algorithm for computing the widths and shifts of spectral lines and, using the definition of the semiempirical Gaunt factor,[5,6] yields Gaunt factors which agree with analytical theory. Experimental bias is minimized since the Stark widths we measure are typically an order of magnitude greater than instrumental and Doppler widths and since electron densities are varied over a substantial range [$(0.3–1.79)\times10^{17}$ cm^{-3}]. An ambiguity in the interpretation of many heavy-element results (whether theoretical uncertainty resides mainly in approximations for interactions or in quantum-mechanical wave functions of the unperturbed ion) is largely avoided by the simple structure (single electron outside of a closed s shell) of Ge II. Line broadening data for some Ge I spectra are also presented. Corresponding predictions are not made, however, because the LS coupling assumed for the model does not necessarily apply to this atom.[7]

II. EXPERIMENT

The spectroscopic shock tube, instrumentation for time-resolved photometry, and techniques for determining plasma conditions have been given in detail elsewhere.[7] Only the more salient features will be summarized here.

The tube ($6.8\times9.3\times510$ cm) is conventional in design and performance. Ambient-temperature hydrogen at 900–1200 lb/in^2 is the driver gas. A variety of test gas mixtures containing germanium hydride, GeH_4, as a minor constituent were used to obtain the ample range of electron densities in the spectroscopic plasmas behind first- and multiply-reflected shock waves. Trial runs were made with various compositions and filling pressure to find useful compromises between signal-to-noise ratios, small optical depths, and photographic exposure. Molar concentrations were 0.6% GeH_4 + 29.4% Ar + 70% Ne, 0.2% GeH_4 + 9.8% Ar + 90% Ne, and 2.0% GeH_4 + 98% Ar.

Earlier experiments[8] using the same apparatus detected no serious systematic departures from homogeneity or local thermodynamic equilibrium (weak diagonal shocks sometimes caused random plasma inhomogeneities and reabsorption in the center of neutral resonance lines accompanied the progressive growth of laminar boundary layers).

Plasma temperatures in most instances were measured simultaneously by three methods: (a) measurement of the reversal intensity[9] at the center of H_α to determine the radiation temperature, (b) and (c) recording of the integrated absolute intensities of H_β and Ne I ($\lambda = 5852$ Å) together with plasma pressures measured via two quartz transducers to determine excitation temperatures[10] for levels of these spectral lines with potentials of 12.7 eV and 18.6 eV, respectively. In the coolest shocks and when neon was not a plasma constituent (8 out of 24 experiments in all), the Ne I ($\lambda = 5852$ Å) line was not usefully bright.

Electron densities were derived from a fit of observed H_β shapes to theoretical Stark profiles[10] and by solving density-compensated Saha relationships.[11] In each experiment, densities determined by these redundant techniques generally agreed to within 20%–25%. This is felt to be commensurate with the random error in fitting Balmer profiles (10%–15%) and with the scatter obtained in temperature and pressure data (3%–5% and 8%–12%, re-

spectively). No significant trends of disagreement between the two types of determination were found. The experimental electron density-temperature regime is shown in Fig. 1.

Germanium line profiles were recorded with a 1-m stigmatic spectrograph using Kodak 103-0 or I-F plates. Pronounced grain of these emulsions limited resolution to 0.3 Å. Exposures of 30–120 μsec were obtained with a fast mechanical shutter.[12] These sampling times were adjusted to correspond to the steady-state duration of the plasma behind first- and multiply-reflected shock waves, which varied according to filling pressures. Multichannel photoelectric photometry (with absolute calibration) carried out in synchronism with the photographic recording[7] provided (1) temperature data, (2) monitors for intensity fluctuations within photographic exposure times,[8] (3) the ability to reconstruct the germanium profiles as they would appear in the optically thin limit.[13]

Spectroscopic emulsions were calibrated with a regulated carbon-arc and various attenuators. Pulsed light sources were used to test for reciprocity failure and adjacency effects—with negative results for spectral densities and exposure times of interest.

Spectroscopic plates were read by a digitizing densitometer, whose output was in turn converted to intensity-versus-wavelength records by a computer code.[13] The typical ratios of signal-to-noise (primarily grain) and of ion linewidth to instrument width are illustrated in Fig. 2.

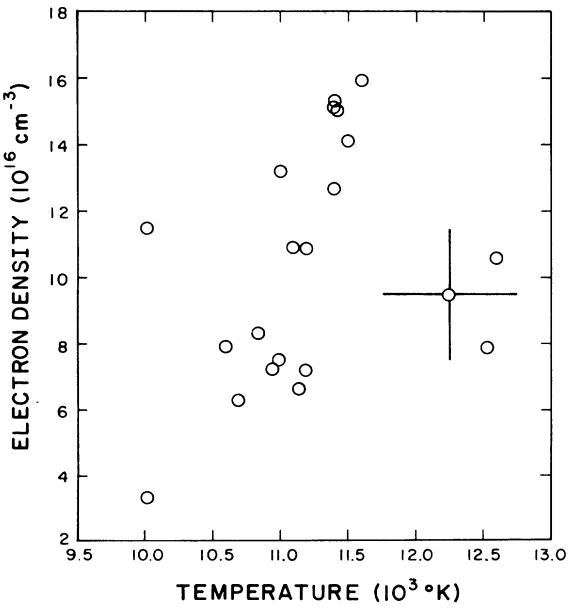

FIG. 1. Experimental temperature—electron-density domain.

To deconvolve experimental profiles into their Stark, instrument, and Doppler components, each intensity profile was digitized at 50–100 points. These profiles were fitted (numerically, in a least-squares sense) to an analytical profile which was a convolution of a Voigt profile and a Fourier representation of the known (measured with various cathodeless discharge lamps) instrument profile.[14] This program assumed a linearly varying continuum, which was indeed consistent with the appearance of the spectra. Since temperatures (Doppler widths) were also known, the fitting of isolated lines involved varying only a single parameter w_l, the Lorentzian component of a Voigt profile. For the blend Ge II ($\lambda = 5178.5$ Å and $\lambda = 5178.6$ Å), the interline separation of the merged pair was also treated as a variable. In this case, the blending introduced little additional uncertainty because the lines have a small (in vacuo) separation compared to their Stark widths (since they belong to the same multiplet, this separation should be maintained by common Stark shifts). The best-fit profile to the data of Fig. 2 illustrates the typical convergence of the fit.

Compensation for the slight ($\simeq 0.1$ Å) Van der Waals broadening contribution to the Lorentzian widths was computed according to the method of Griem.[15] The majority of profiles were obtained at 11 000 °K ± 10%; thus calculated adjustments for the dependence of impact broadening on temperature[2] were very small.

III. THEORY

Within the temperature-density regime of Fig. 1, Stark broadening is dominated by electron-impact broadening,[2] with ionic perturbers estimated in the quasistatic approximation to contribute less than 5% to the Ge II linewidths. We therefore follow the usual semiclassical approach[4] and calculate

$$w + id = \langle if || \sum_j f_j (1 - S_{ij} S_{fj}^{\dagger}) || if \rangle ,$$

where i, f are the initial and final states, respectively, $||if\rangle$ is a wave function in "doubled" line space, and $\sum_i f_i$ averages over impact parameters and the velocity distribution. The calculation involves making a perturbation expansion of $\tilde{S}$, the matrix for scattering of electrons by ions, and retaining only the leading terms.[16] We denote by w the half-width, which is one-half of the separation between half-intensity points, and by d the shift, which is the separation of the profile maximum from the unperturbed profile ($N_e \to 0$).

Incomplete classification of close-lying perturbing levels is considered to be the major source of

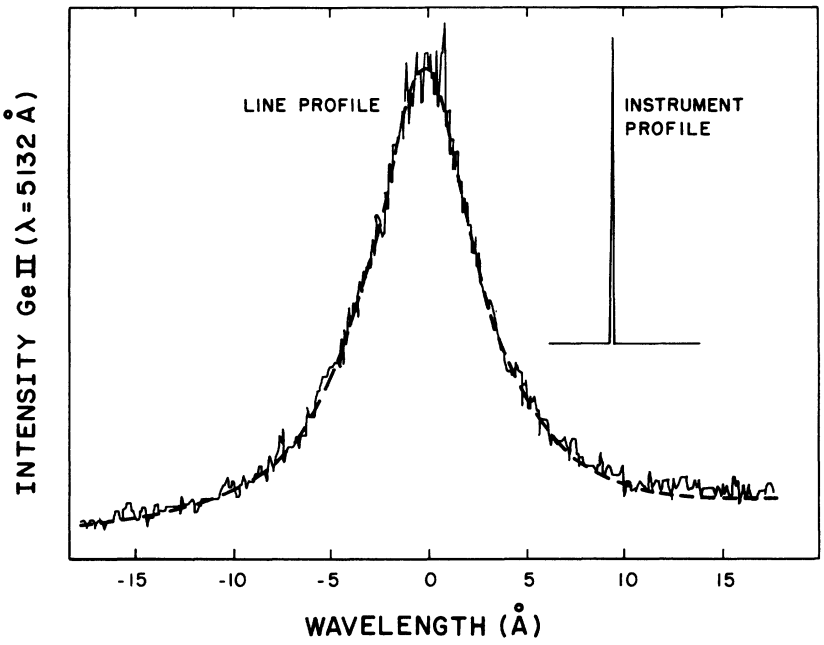

FIG. 2. Typical intensity-versus-wavelength data, illustrating signal-to-noise ratios and the relative widths of instrumental and Ge II line profiles. The superimposed broken curve represents the best-fit Voigt shape, including instrument broadening.

error in the semiclassical treatment, with uncertainties in the dipole oscillator strengths and energy levels contributing to a lesser extent. By way of sensitivity analysis, predictions for Ge II lines were made using experimental "f" values[17] and alternatively, oscillator strengths calculated to reduce $\Delta S/S$ (see Sec. IV) to zero.[4,18] Although the differences between these two sets of oscillator strengths were as much as a factor of 2, Stark widths based on the two types of data differed by less than 5%. The calculated widths are shown in Table I.

No attempt was made to calculate the Stark widths of the two measured Ge I lines because the *LS* coupling inherent in our computer codes is not appropriate to this stage of ionization.[17,19]

IV. RESULTS AND DISCUSSION

Experimental results are compared with theory in Table I. Stark widths are normalized to an electron density of 10^{17} cm^{-3} and a temperature of 11 000°K. Tabulated uncertainties are 67% confidence limits, based on statistical analysis of between 8 and 24 profiles (the number of profiles used for the statistical analysis of each line is shown in Table I) and best estimates of possible bias. The observed scatter in the broadening parameters, typically 25%, is commensurate with our

TABLE I. Comparison of measured and calculated Stark widths of Ge I and Ge II. The definitions of $\Delta S/S$, $\bar{g}$, and kT/E are explained in Ref. 4. The wavelength and the half-widths (w) are in angstroms. w_1 is the width for each component of the multiplet and N_1 is the number of profiles used to obtain this value, w_m is the corresponding average value, and w_c is the calculated width using the semiclassical algorithm. The widths are normalized to $N_e = 10^{17}$ cm^{-3} and are corrected for other broadening mechanisms.

Ion	Multiplet	λ	w_1	N_1	w_m	w_c	$\Delta S/S$	$\bar{g}$	kT/E
II	$4d\,^2D$-$4f\,^2f$	5131.8	2.27	9	2.37±10%	2.32	−0.35	0.39	34.0
		5178.5	2.42	11					
		5178.6	2.42	11					
II	$5p\,^2P$-$4d\,^2D$	4815.6	3.10	8	2.98±10%	3.03	−0.08	0.17	34.0
		4741.8	2.75	9					
		4824.1	3.10	8					
II	$5s\,^2S$-$5p\,^2P$	5893.4	2.61	13	2.13±10%	1.22	−0.47	0.49	4.1
		6021.0	1.64	15					
I	$4p\,^1D$-$5s\,^3P$	4684.8		1	0.35±30%				
I	$4p\,^1S$-$5s\,^1P$	4226.5		1	3.18±30%				

estimates of (20–25)% random error in electron density and 5% in grain noise per profile reading.

The parameter $\Delta S/S$ appended to the theoretical widths is a gauge of the completeness of the set of utilized perturbing levels and it is analogous to the f sum for dipole transitions. A $\Delta S/S$ approaching zero implies that essentially all allowed perturbing levels have been accounted for. Generally, $\Delta S/S < 0.4$ corresponds to good agreement of predictions with experiment.[4]

The most striking features of the table are: first, the excellent agreement between measured and calculated widths for the multiplets $4d\,^2D$-$4f\,^2F$ and $5p\,^2P$-$5d\,^2D$ as well as the agreement within the multiplets due to fine-structure splitting; secondly, the disagreement found for the $5s\,^2S$-$5p\,^2P$ multiplet both in comparing theoretical with measured values and intramultiplet broadening. This latter disagreement contrasts sharply with our other Ge II data as well as previous measurements of similar atomic systems.[4]

There are several possible mechanisms which could cause this discrepancy: First, if we assume that LS coupling is valid for this ion (which should be the case), then the only distinction between lines profiles within a multiplet should be the λ^2 dependence of the widths.[2,15,16] Results for this multiplet are shown in Fig. 3 and the range of experimental values clearly falls outside of the theoretical estimates. Secondly, it is possible that LS coupling is not valid for one or more of the energy levels of this ion. This is belied by the other width measurements of this experiment and a previous experiment[17] which measured the A values and found good agreement between experimental and theoretical (Coulomb approximation) predictions as well as consistency in J-file and f-sum rules. Normally A values are more sensitive to correctness of energy and angular momentum than are the Stark widths, so we would expect this second experiment to be an even better test of LS coupling. Thirdly, there is the possibility that one or more perturbing levels have been assigned the wrong energy. Since theory and experiment agree for the other profiles, it would have to be a level which is very close to the $5s\,^2S$, lower in energy and which affected only this multiplet (even this would not explain the intramultiplet differences). There is no simple means (other than that used to classify the levels initially[19]) to check on this possibility. Fourthly, both spectral lines would appear broader if there were impurity lines underlying the lines of interest. The only possibility is the C II (5) multiplet at 5889.2 and 5891.7 Å. This possibility is ruled out, however, by the absence of C I and C II lines elsewhere in the spectrum; finally, neither spectral line was optically thick, which can be ascertained directly from the data reduction and from the simple linear dependence of the ratios of the intramultiplet Stark widths seen in Fig. 3.

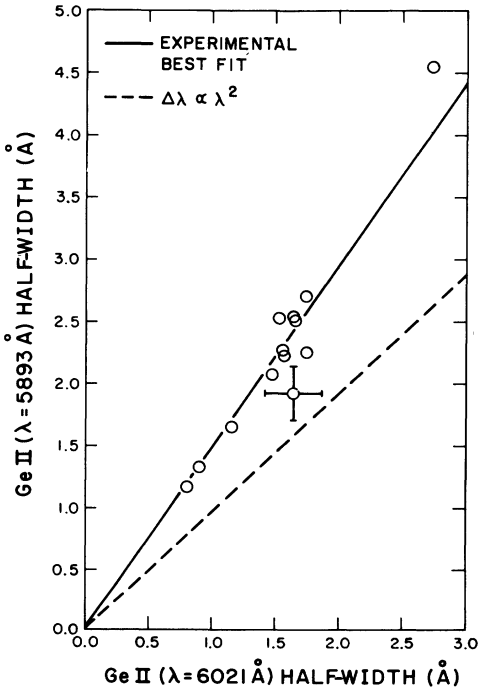

FIG. 3. A comparison of the Stark widths of the $5s\,^2S$-$5p\,^2P$ multiplet of Ge II ($\lambda_0 = 5893.4$ Å and $\lambda_0 = 6021.0$ Å). Also plotted is the expected correlation between the two spectral lines, assuming LS coupling is valid.

V. CONCLUSION

We thus conclude that the relatively simple semiclassical algorithm is of sufficient accuracy (±20%) for width, shift, and opacity calculations, even for heavy atomic systems which heretofore have had no measurements or calculations done for them. The one anomaly for which the calculations do not agree with the measurements is also not self-consistent within the multiplet and thus should not be used as a basis for comparison.

ACKNOWLEDGMENTS

This research was supported in part by National Aeronautics and Space Administration grants No. NGR 21-002-007/9 and NGR 44-012-258. Computer time was furnished through the Computer Science Center of the University of Maryland under a grant from the National Aeronautics and Space Administration, No. NSG-398. The authors wish to acknowledge the encouragement of Dr. T. D. Wilkerson and Dr. H. R. Griem and the assistance of J. A. Griffith, J. Clawson, and R. Roig in the reduction of the data.

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