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DATA REDUCTION IN RUBY LUMINESCENCE EXPERIMENTS

PAUL HORN

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Shock Dynamics Laboratory

Department of Physics

Washington State University

Pullman, WA 99164

In the reduction of spectroscopic data, it is generally necessary to determine the wavelengths of spectral peaks. In the case of the ruby R-lines, these peaks are relatively sharp (especially at low temperature), while in other cases, such as the ruby absorption bands, they are broad. When the peaks are sufficiently sharp and well resolved, there are several methods which can be used to determine their wavelengths; however, care should be taken when comparing the results of alternate methods to insure that systematic differences do not exist between the quantities so determined. For example, one may define either the maximum of a peak or its centroid as the peak location, but values obtained from these definitions may be different for asymmetric peaks. Different methods of peak location and of wavelength calibration of the recording system were used by Jim Burt in his experiments on ruby at low temperature than were used in the room temperature and low temperature tension experiments. The purpose of this note is to discuss any systematic differences between these results.

In the room temperature and tension data, the R-line positions were determined graphically by using the SDL program IPL. This routine displays densitometer format images, and provides a crosshair for locating image features. The crosshair step size corresponds to approximately 1 pixel for a 500 pixel OMA image, which is equivalent to 0.4 Å at the typical dispersion of 0.4 Å/pixel employed in the room temperature experiments. The centroid of the peak (equal area on either side of the crosshair) was taken to be the peak position. In order to obtain a wavelength calibration, given only the two R-lines as standards, several reference spectra were recorded at various settings of the spectrograph wavelength selector. The final reference was recorded at the setting used in the experiment. The accuracy of this technique relies on the accuracy of the spectrograph drive mechanism, but it should be reasonably good over the small wavelength range observed ($\approx$ 200 Å). The room temperature data were obtained on the Cordin streak system, and calibrations were recorded in the focus mode (i.e. not streaked) at the center of the detector window. Tests of the Cordin system did not exhibit curvature in streak images, which would have necessitated calibration over the whole streak length; however, in general a streak calibration is preferable and that is the method used in the tension experiments performed with the Imacon streak system.

The method used by Jim Burt in the low temperature compression experiments differed both in the calibration procedure and the peak location. Peak positions were chosen to be the maximum obtained in a quadratic least squares fit to a portion of the peak. This automates the procedure, but only works for clean, well defined peaks. The computer routine used was unable to analyze a typical room temperature record. The calibration differed from the procedure used in the room temperature experiments in that only two calibration wavelengths were recorded, those being the low temperature R-lines. This eliminates errors due to the spectrograph drive, but is much more sensitive to errors in locating the calibration peaks and specifying the ambient wavelengths. Also the calibration must be extrapolated to determine the red-shift of the R_1 line (the R_2 line in the elastic range lies within or near the calibration range).

Comparison of data

All of the existing data are plotted in Figures 1 and 2 for R_1 and R_2 respectively. The circle symbols denote the room temperature and tension data, and the triangles represent the low temperature compression data. The solid lines are quadratic least squares fits to the room temperature and tension data, with the constraint of zero wavelength shift at zero density compression. The agreement is good, even though the low temperature compression data were not included in the fit. For completeness, I have performed a statistical comparison based on the technique of normal probability plots described by Abrahams and Keve.[1] In this method, the measured deviations between two sets of values are ordered from smallest (or most negative) to largest and compared with the most probable deviations for the given number of values and the assumed error distribution (in this case Gaussian). If the errors are so distributed, the two sets of values correctly scaled, and the standard deviations correctly estimated, a plot of measured deviations against expected deviations yields a straight line passing through the origin of unity slope. A non-linear plot indicates systematic error, while a slope other than unity indicates incorrect estimation of the standard deviation in the data.

I have compared each set of data with the quadratic fit to look for systematic differences. The normal probability plots are presented in Figures 3 and 4. Both plots appear to be roughly linear with slopes of approximately one. This indicates that no large systematic error exists and that the chosen standard deviations are appropriate (0.4 Å for the room temperature and tension data, 0.3 Å for the low temperature compression data). Both plots show an offset from the origin, -0.2 Å (0.5 standard deviations) for the room temperature/tension and +0.3 Å for the low temperature compression. This would normally indicate an incorrect scale factor, which should not occur in a least squares fit. The -0.2 Å offset in the early data is most likely due to inability of the constrained quadratic fit to fully accommodate the data. The +0.3 Å offset of the latter data then indicates a small, but statistically notable difference in the data sets.

Comparison of methods

In order to determine the differences engendered by the two analysis methods, two experimental records (one from each set) were reanalyzed according to alternate techniques. The low temperature experiment 87-533 was processed using the IPL routine to locate peaks. The corresponding calibration method could not be applied as the necessary data were not recorded. Using only the two available calibration points, I obtained wavelength shifts of 18 Å (R_1) and 19.7 Å (R_2), as compared to the previous values of 17.3 Å and 19.6 Å The routine employed for analyzing low temperature data was not successful in processing a room temperature record, however, applied to tension experiment 88-506 it reproduced the wavelength values to within 0.6 Å

A reanalysis of all of the records would be required to determine whether the differences observed above account for the systematic variation seen in the normal probability plots. I do not believe that such an endeavor is warranted as the differences are on the order of the experimental error. I recommend that a standard method be adopted for future ruby experiments as follows:

1. More than two calibration points should be recorded, whether by identifying additional sources or by varying the spectrograph setting. The range of calibration should not be extrapolated by a factor of two.

2. Peak positions should be chosen by a systematic technique suitable for noisy records as well as clean ones. One such method would be to numerically integrate to determine the centroid. The results should be checked graphically.

I believe that these considerations will become increasingly important as the ruby technique is refined for better stress resolution, especially in fast measurements of wave profiles.

REFERENCES

1. S.C. Abrahams and E.T. Keve, "Normal probability plot analysis of error in measured and derived quantities and standard deviation", Acta Cryst., *A27,* 157 (1971).

FIGURE CAPTIONS

FIG. 1. R_1 wavelength shift. The circle symbols indicate room temperature and tension data. The triangles correspond to low temperature compression data. The solid line is the result of a quadratic least squares fit of the room temperature and tension data.

FIG. 2. R_2 wavelength shift. The square symbols indicate room temperature and tension data. The triangles correspond to low temperature compression data. The solid line is the result of a quadratic least squares fit of the room temperature and tension data.

FIG. 3. Normal probability plot comparing room temperature and tension data with quadratic fit.

FIG. 4. Normal probability plots comparing low temperature compression data to quadratic fit of room temperature and tension data.