TEMPERATURE DETERMINATION OF SHOCK LAYER USING SPECTROSCOPIC TECHNIQUES

Final Report

NASA/ASEE Summer Faculty Fellowship Program -- 1989

Johnson Space Center

Prepared BY: Murty A. Akundi, Ph.D.
Academic Rank: Associate Professor
University & Department: Xavier University
Physics/Engineering Department
New Orleans, Louisiana 71245

NASA/JSC
Directorate: Engineering
Division: Structure and Mechanics Division
Branch: Thermal
JSC Colleague: John E. Grimaud
Date Submitted: August 11, 1989
Contract Number: NGT 44-001-800
ABSTRACT

Shock layer temperature profiles are obtained through analysis of radiation from shock layers produced by a blunt body inserted in an arc jet flow. Spectral measurements of $N_2^+$ have been made at $0.5''$, $1.0''$ and $1.4''$ from the blunt body. A technique is developed to measure the vibrational and rotational temperatures of $N_2^+$. Temperature profiles from the radiation layers show a high temperature near the shock front and decreasing temperature near the boundary layer. Precise temperature measurements could not be made using this technique due to the limited resolution. Use of a high resolution grating will help to make a more accurate temperature determination. Laser induced fluorescence technique is much better since it gives the scope for selective excitation and a better spacial resolution.
INTRODUCTION

Temperature determination of the shock layer during the space vehicle reentry conditions is of utmost importance for thermal protection system (TPS). The identification, characterization and temperature determination of different atomic, molecular and ionic species in the shock layer and boundary layers form the basis of the plasma diagnostics program in the atmospheric reentry materials and structures evaluation facility (ARMSEF). Vibrational and rotational temperature determinations were made for \( \text{N}_2 \) and \( \text{N}_2^+ \) by Blackwell et. al. (1). Their technique involves calculating the spectrum for a number of cases and obtain integrals over the wavelength regions of the spectrum as functions of temperature. Ratios of these integrals were then related to the temperatures used to generate the spectra. Spectral integrals from measured spectra were then compared with the calculated values to determine the temperature. This technique has some limitations and needs lot of parameters to produce the calculated spectra. In this report I will present a simple technique to find the vibrational and rotational temperatures of molecules in the shock layer which in turn can be related to the temperature of the shock layer.

MEASUREMENTS

Facility:

A lay out of the experimental set up is shown in fig. 1. Mixture of \( \text{N}_2 \) and \( \text{O}_2 \) are heated in an arc powered by a variable direct current power supply. The hot discharge products (Plasma) are then expanded through a conical nozzle which gives hypersonic speeds to the plasma. A shock layer is formed when a thermal protection system (TPS), for example a tile, is introduced in this flow. One of the major criteria at the NASA/JSC arc jet facility is to understand the heat transfer process to TPS. Rotational temperature determination of molecular species is one of the major parameters, since this temperature is close to the shock layer temperature. This is achieved by spectroscopic techniques which are non intrusive in nature.

Spectral system:

Light emitted from the shock layer of a blunt body is focused on to an entrance slit of 0.6m SPEX triplemate spectrometer having 1024 linear diode array detector. A 600 lines/mm and 1800 lines/mm gratings were used, yielding a pixel resolution of 0.069nm and 0.023nm respectively.

1-3
The spectral data were recorded using an optical multichannel analyzer (OMA) system, on which the wavelength and intensity calibrations are performed and integrations may be made.

$N_2^+$ spectra between 340 nm and 480 nm at 0.5" from the blunt body using 600 lines/mm grating is shown in fig. 2. This low resolution spectra was used to find the vibrational temperature. Rotation structure of 0-1 band taken on 1800 lines/mm grating at various distances from the blunt body are used for rotational temperature determinations.

RESULTS AND ANALYSIS

Vibrational temperature of a given vibrational state can be obtained theoretically (2) using

$$\ln \left[ \frac{I(v',v'')}{v'^4} \right] = c_1 - G'(v') \frac{hc}{kT} \quad (1)$$

where

- $c_1 = \text{a constant}$
- $G'(v') = w_e'(v' + .5) - w_e'x_e'(v' + .5)^2$
- $w_e'$ and $w_e'x_e'$ values are taken from Huber and Herzberg (3)
- $h = \text{Planck's constant}$
- $c = \text{Speed of light}$
- $k = \text{Boltzmann's constant}$
- $T = \text{the temperature to be determined}$

By plotting a graph of logarithm of the intensities of the progressions against the vibrational term ($G(v)$), a straight line is obtained. The slope of the line gives $hc/kT$ from which the vibrational temperature of a given electronic state can be determined. This method is used for the spectra taken at 0.5" from the blunt body and is shown in fig.2. The areas under the curves of 0-1, 1-1, 2-1, and 3-1 bands of the $N_2^+$ were used for vibrational temperature determinations. The graph along with the calculated temperature is shown in fig.3. The temperature determined using this technique is close to the one determined earlier by Blackwell et.al (1) at this distance. Vibrational temperature determinations using other progressions could not be made as sufficient data is not available. This procedure seems to be simple and
comparable to the methods used by earlier workers (1).

During my stay here, more emphasis is given for rotational temperature determinations of $N_2^+$. The necessary equations for determining the rotational line intensities are shown in Appendix 1. When a graph is plotted using equation (4) between $\ln \left[ I/(k'+k''+l) \right]$ against $k'(k'+1)$, a straight line is obtained. The slope of the line gives $B_0hc/kT$ from which the rotational temperature can be determined.

The rotational structure of the 0-1 band of $N_2^+$ is shown in fig.4. Due to the limited resolution the spectrum is not well resolved and we could not resolve P and R branches. As a first order approximation, we tried to treat the observed peak intensity as purely due to the P branch only and rotational temperature determinations are made as per equation (4) shown in Appendix 1. Similarly considering the observed intensity as purely due to the R branch, rotational temperature is determined. As shown in fig.5, the temperatures obtained are not the same and not close to the rotational temperatures determined by earlier methods(4). this is expected because the experimental spectra contains the intensity contributions of both P and R branches. One therefore cannot use equation (4) for cases where the spectra are not well resolved.

We have developed a method to determine the rotational temperatures in cases where the P and R branches are not well resolved. The necessary equations have been derived and shown in Appendix 2. Using equations (7) and (8) the observed intensity is corrected for P and R branches at various temperatures(T). Graphs are now plotted; $\ln[I_{PC}/(K'+K''+1)]$ against $K'(K'+1)$ for P- branch and $\ln[I_{RC}/(K'+K''+1)]$ against $K'(K'+1)$ for R-branch. The temperatures ($T_P$ and $T_R$) are now calculated using the slopes of the straight lines obtained from the graphs for both P and R branches. The particular set for which the temperature $T_P = T_R = T$ is considered as the temperature of the shock layer.

Using this method, spectra taken at 0.5", 1.0" and 1.4" from the blunt body on October '88 are analyzed for rotational temperature determination. Figs. 6 and 7 show the graphs plotted for the corrected P and R branches at various temperatures for the spectra taken at 0.5" from the body. Temperatures are calculated using the slopes of the lines and are tabulated in Table 1. The best agreement is obtained at 5000 K as can be seen from the % errors shown in Table 1. Fig. 8 is a graph showing the agreement between P and R branches. Similar calculations are carried out for spectra.
taken at 1.0" and 1.4" and the corresponding temperatures are found to be 6000 K and 5000 K respectively.

CONCLUSIONS

We have developed a procedure to calculate the vibrational and rotational temperatures of simple molecules. These methods have been tested to determine the shock layer temperatures of N$_2^+$ and it could be extended to other molecular species present in the shock layer. We encountered some problems of convergence when the rotational temperature procedure was tested on a different data set. This therefore needs further testing with bigger data base. The accuracy of rotational temperature determination could be improved further if the P and R branches could be resolved.

Recommendations: In order to obtain a more accurate temperature determination and to resolve P and R branches the following Suggestions are made.

1. A bigger spectrometer of at least one meter in length with 1800 lines/mm will be able to resolve the spectra.

2. A photodiode array with five times the present photodiode density will basically also resolve the spectra.

3. Laser Induced fluorescence on the other hand will provide selective excitation, spatial as well as high resolution. Therefore this seems to be the ideal approach for the present problem.
ACKNOWLEDGMENTS

I wish to take this opportunity to thank NASA/ASEE summer faculty fellowship program for giving me an opportunity to work at NASA, Johnson Space center. My sincere thanks are to John Grimaud, my NASA colleague, for providing the facilities and for his complete cooperation. My special thanks are to Dr. Sivaram Arepalli of Lockheed without whose help I might not have been able to complete this work. Last but not the least, I wish to thank all NASA and the Lockheed personnel of the arc jet facility who made my stay here very pleasant and rewarding.
REFERENCES


EXPERIMENTAL ARRANGEMENT

Fig. 1
Nirogen Molecular Ion, Vibrational Spectrum

Fig. 2.
Vibrational Temperature of Nitrogen molecular ion
0.5", 600 amp

Fig. 3
Nitrogen Molecular Ion (0,1) band, Rotational structure
Nitrogen Molecular Ion (0,1) band, 0.5", 800amp

\[
\ln\left(\frac{1}{(K'+K''+1)}\right) \quad \text{vs} \quad K'(K'+1)
\]

- \( \bigcirc R- \text{ branch}(860 \text{ K}) \)
- \( \bigtriangleup P- \text{ branch}(15,500 \text{ K}) \)

Fig. 5.

10/24/88
Nitrogen Molecular Ion (0,1) band, 0.5", 800 amp
P–branch

\[ \ln \left( \frac{1}{(K' + K'' + 1)} \right) \]

\[ K'(K' + 1) \]

\[ 1000 \text{ K} \]
\[ 3000 \text{ K} \]
\[ 4000 \text{ K} \]
\[ 5000 \text{ K} \]
\[ 6000 \text{ K} \]
\[ 8000 \text{ K} \]
\[ 10000 \text{ K} \]

Fig. 6
Nitrogen Molecular Ion (0,1) band, 0.5", 800 amp
R-branch

$\ln\left[\frac{1}{(k'+1)}\right]$ vs. $k'(k'+1)$

Fig. 7
Nitrogen Molecular Ion (0,1) band; 0.5", 800 amp
TABLE I

NITROGEN MOLECULAR ION
(0,1) BAND, 0.5", 800 AMP

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Temperature (K)</th>
<th>% Error</th>
<th>Temperature (K)</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actual</td>
<td>R-Branch</td>
<td></td>
<td>P-Branch</td>
<td></td>
</tr>
<tr>
<td>1,000</td>
<td>1,820</td>
<td>82</td>
<td>1,188</td>
<td>19</td>
</tr>
<tr>
<td>3,000</td>
<td>5,124</td>
<td>71</td>
<td>3,497</td>
<td>17</td>
</tr>
<tr>
<td>4,000</td>
<td>5,091</td>
<td>27</td>
<td>4,276</td>
<td>7</td>
</tr>
<tr>
<td>5,000</td>
<td>4,874</td>
<td>2.5</td>
<td>4,860</td>
<td>2.8</td>
</tr>
<tr>
<td>6,000</td>
<td>4,629</td>
<td>22</td>
<td>5,288</td>
<td>12</td>
</tr>
<tr>
<td>8,000</td>
<td>4,304</td>
<td>46</td>
<td>5,912</td>
<td>26</td>
</tr>
<tr>
<td>10,000</td>
<td>4,104</td>
<td>59</td>
<td>6,307</td>
<td>37</td>
</tr>
</tbody>
</table>
APPENDIX - 1

ROTATIONAL TEMPERATURE EQUATIONS

\[ I(P - \text{Branch}) = A - 2J e^{- \frac{B_0 J(J - 1) \hbar c}{kT}} \]

(1)

\[ I(R - \text{branch}) = A - 2(J + 1) e^{- \frac{B_0 (J + 1)(J + 2) \hbar c}{kT}} \]

(2)

Rearranging equations (1) and (2)

\[ \ln \left( \frac{I_p}{2J} \right) = \ln A - \frac{B_0 J(J - 1) \hbar c}{kT} \]

\[ \ln \left( \frac{I_p}{2J} \right) = A' - \frac{B_0 J(J - 1) \hbar c}{kT} \]

(3)

Similarly for R Branch

\[ \ln \left( \frac{I_R}{2(J + 1)} \right) = A' - \frac{B_0 (J + 1)(J + 2) \hbar c}{kT} \]

(4)

Equation (3) and (4) can general be written for either case as

\[ \ln \left( \frac{I}{k' + k'' + 1} \right) = A - \frac{B' K'(k' + 1) \hbar c}{kT} \]

where $k'$ - upper rotational state quantum number

$k''$ - lower rotational state quantum number
CORRECTED INTENSITIES

\[ I_{\text{EXP}} = I_P + I_R \]  \hspace{1cm} (5)

\[ \frac{I_{\text{EXP}}}{I_R} = \frac{I_P}{I_R} + 1 \]  \hspace{1cm} (6)

Let \( \frac{I_P}{I_R} = B \) where \( I_P \) and \( I_R \) are the intensities calculated for any temperature using equations (1) and (2)

\[ I_{Rc} = I_{\text{EXP}} \left[ \frac{1}{1 + B} \right] \]  \hspace{1cm} (7)

\[ I_{Pc} = I_{\text{EXP}} \left[ \frac{1}{1 + \frac{1}{B}} \right] \]  \hspace{1cm} (8)

\( I_{Rc} \) and \( I_{Pc} \) are the intensity contributions of \( P \) and \( R \) branches in the observed spectra.