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Ionization Cross Sections for "After 2 Days" RGA Spectrum

1 Purpose

To calculate electron-impact ionization cross sections for gas species found in the "After 2 Days" residual gas analyzer (RGA) spectrum taken on 5/21/18. The spectrum was analyzed using gnuplot and is shown below in Figure 1. Each substantial peak was identified and fit with a Gaussian function in order to determine the partial pressures of the various species of residual gas in the gun chamber. NOTE: The peak values must be divided by the correction factors listed here: https://www.mksinst.com/docs/ur/GaugeGasCorrection.aspx

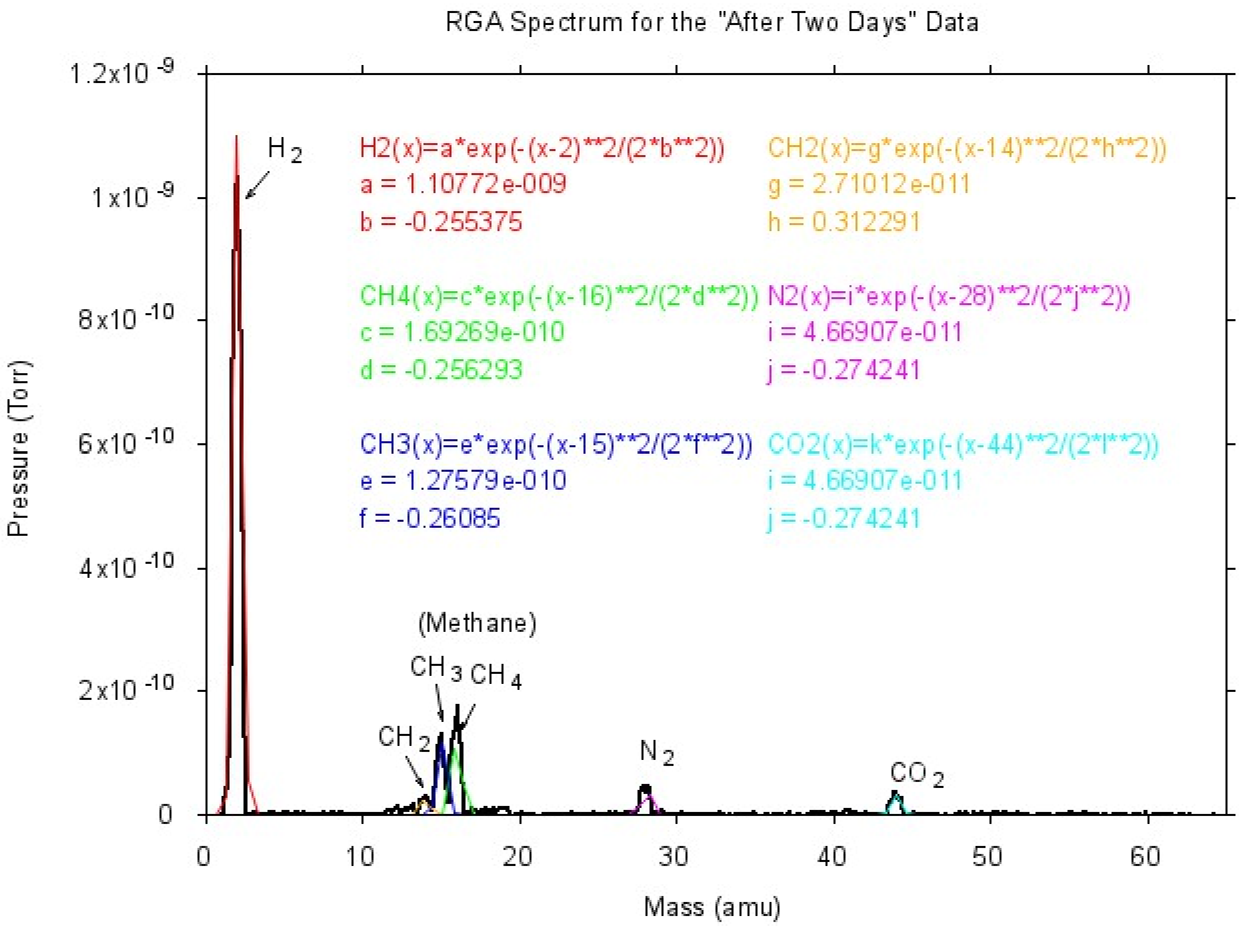

Figure 1: Analysis of the RGA spectrum for the "After 2 Days" data (before correction factor)

2 Calculation of the Ionization Cross Section

The equation for the calculation of the ionization cross section σ_i of the i^{th} gas species can be found in Reiser [1] and was originally developed by Slinker et. al. [3]:

$$\sigma_i = \frac{8a_0^2 \pi I_R A_1}{m_e c^2 \beta^2} f(\beta) \left(\ln \frac{2A_2 m_e c^2 \beta^2 \gamma^2}{I_R} - \beta^2 \right) \tag{1}$$

Numerically, this can be rewritten as:

$$\sigma_{i[\mathrm{m}^2]} = \frac{1.872 \times 10^{-24} A_1}{\beta^2} f(\beta) \left[\ln\left(7.515 \times 10^4 A_2 \beta^2 \gamma^2\right) - \beta^2\right] \tag{2}$$

In these two equations, $a_0 = 5.29 \times 10^{-11}$m is the Bohr radius, $I_R = 13.6$eV is the Rydberg energy, $m_e c^2$ is the rest mass energy of the electron, and β and γ are relativistic factors, A_1 and A_2 are empirical constants that depend on the type of gas species, and $f(\beta)$ is a function used when fitting data at low energies, i.e. $T_e \approx I_i$ where T_e is the kinetic energy of the elctron and I_i is the ionization energy for the i^{th} gas species. Expressions for A_1, A_2, and $f(\beta)$ are given below:

$$f(\beta) = \frac{I_i}{T_e}\left(\frac{T_e}{I_i} - 1\right) = \frac{2I_i}{m_e c^2 \beta^2}\left(\frac{m_e c^2 \beta^2}{2I_i} - 1\right) \tag{3}$$

$$A_1 = M^2 \tag{4}$$

$$A_2 = \frac{e^{\frac{C}{M^2}}}{7.515 \times 10^4} \tag{5}$$

where C and M^2 are parameters given by Rieke and Prepejchal [2]. For H_2, CH_4, CH_3, N_2, and CO_2 the values of C, $M^2 = A_1$, A_2, and the ionization energy I_i from NIST (https://webbook.nist.gov/) are given in the table below:

Gas Species	$A_1 = M^2$	C	A_2	I_i(eV)
H_2	0.695	8.115	1.5668	15.4
CH_4	4.23	41.85	0.2635	12.6
N_2	3.74	34.84	0.1478	15.6
CO_2	5.75	55.92	0.2227	13.8

Table 1: Values for C, $M^2 = A_1$, and A_2 given by Rieke and Prepejchal and I_i given by NIST for gas species found in the RGA spectrum.

Since at high energies, $\beta_e \gg \beta_{ion}$, we will assume that in the above equations, $\beta \approx \beta_e$. As an example calculation, for a 200keV electron beam, $T_e = 200$keV, $m_e c^2 = 511$keV, the cross section for H_2 gas is:

$$\begin{aligned}
T_e &= (\gamma_e - 1) m_e c^2 = 200\text{keV} \\
m_e c^2 &= 511\text{keV} \\
\gamma_e &= 1 + \frac{T_e}{m_e c^2} = 1.39 \\
\beta_e &= \sqrt{1 - \frac{1}{\gamma_e^2}} = 0.695 \left(= 2.08 \times 10^8 \frac{\text{m}}{\text{s}}\right) \\
f(\beta_e) &= \frac{I_i}{T_e}\left(\frac{T_e}{I_i} - 1\right) \approx 1 \\
\sigma_i &= \frac{1.872 \times 10^{-24} A_1}{\beta_e^2} f(\beta_e) \left[\ln\left(7.515 \times 10^4 A_2 \beta_e^2 \gamma_e^2\right) - \beta_e^2\right] \\
&\approx 2.994 \times 10^{-23}\text{m}^2
\end{aligned}$$

3 Ionization Rate

The change in density of the electron and gas molecules over time is given by Reiser[1]

$$\frac{dn}{dt} = n_b n_g \sigma_i v = n_b n_g \sigma_i \beta_e c \tag{6}$$

At standard temperature ($T_0 = 273.15\text{K}$) and pressure ($p_0 = 760\text{torr} = 1\text{atm}$) the density of an ideal gas in a given volume is given by Loschmidt's number:

$$n_0 = \frac{p_0}{k_B T_0} \approx 2.687 \times 10^{25}\text{m}^{-3} \tag{7}$$

Thus, for a given gas, its density is

$$n_g\left[\text{m}^{-3}\right] = \left(3.54 \times 10^{22}\right) p\,(\text{torr})$$

For H_2, $p\,(\text{torr})$ can be read off from Figure 1. In this case, $p_{H_2} = 1.11 \times 10^{-9}\text{torr}$ with a correction factor of 0.46 for H_2, so $n_{H_2} = 8.54 \times 10^{13}\text{m}^{-3}$. Knowing the electron density in the beam, n_b, one can calculate the ionization rate $\frac{dn}{dt}$. For a numerical example, assume we have a 200keV, 1mA uniform, cylindrical electron beam with an average transverse size of 1mm. In this case, $T_e = 200\text{keV}$, $I = 1\text{mA}$, $\sigma_{H_2} = 2.994 \times 10^{-23}\text{m}^2$, and $n_b \approx 1.98 \times 10^{21}\text{m}^{-3}$. Then for H_2,

$$\begin{aligned}
\frac{dn_{H_2}}{dt} &= n_{H_2} n_b \sigma_{H_2} \beta_e c \\
&= \left(8.54 \times 10^{13}\text{m}^{-3}\right)\left(1.98 \times 10^{21}\text{m}^{-3}\right)\left(2.994 \times 10^{-23}\text{m}^2\right)(0.695)\left(2.998 \times 10^8\frac{\text{m}}{\text{s}}\right) \\
&\approx 1.05 \times 10^{21}\text{m}^{-3}\,\text{s}^{-1}
\end{aligned}$$

4 Ionization Cross Section vs. T_e

Starting from equation (2),

$$\sigma_i\left[\text{m}^2\right] = \frac{1.872 \times 10^{-24} A_1}{\beta^2}\frac{I_i}{T_e}\left(\frac{T_e}{I_i} - 1\right)\left[\ln\left(7.515 \times 10^4 A_2 \beta^2 \gamma^2\right) - \beta^2\right]$$

we can rewrite β in terms of the electron beam kinetic energy T_e, which is proportional to the beam voltage:

$$\begin{aligned}
T_e &= (\gamma - 1)\, m_e c^2 \\
\gamma &= 1 + \frac{T_e}{m_e c^2} \\
\frac{1}{\sqrt{1-\beta^2}} &= 1 + \frac{T_e}{m_e c^2} \\
1 - \beta^2 &= \left(\frac{1}{1 + \frac{T_e}{m_e c^2}}\right)^2 = \left(\frac{m_e c^2}{m_e c^2 + T_e}\right)^2 \\
\beta^2 &= 1 - \left(\frac{m_e c^2}{m_e c^2 + T_e}\right)^2
\end{aligned}$$

Thus,

$$\sigma_i = \frac{1.872 \times 10^{-24} A_1}{1 - \left(\frac{m_e c^2}{m_e c^2 + T_e}\right)^2}\frac{I_i}{T_e}\left(\frac{T_e}{I_i} - 1\right)\left[\ln\left(7.515 \times 10^4 A_2\left(1 - \left(\frac{m_e c^2}{m_e c^2 + T_e}\right)^2\right)\left(1 + \frac{T_e}{m_e c^2}\right)\right) - \left(1 - \left(\frac{m_e c^2}{m_e c^2 + T_e}\right)^2\right)\right]$$

Using values in Table 1, a plot of σ_i vs. T_e for each of the gas species was made using Mathematica:

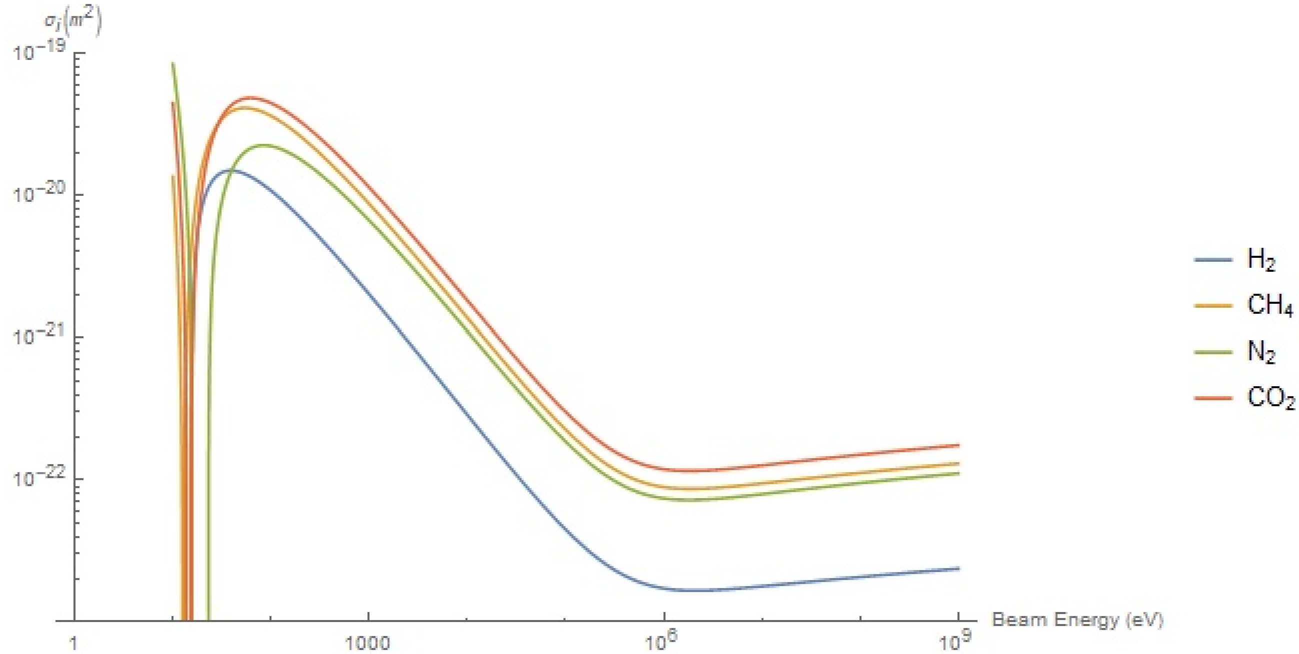

Figure 2: Plot of the ionization cross section σ_i vs. electron kinetic energy T_e

References

[1] Martin Reiser. *Theory and Design of Charged Particle Beams.* Wiley VCH Verlag GmbH, 2008.

[2] Foster F. Rieke and William Prepejchal. Ionization cross sections of gaseous atoms and molecules for high-energy electrons and positrons. *Physical Review A*, 6(4):1507–1519, oct 1972.

[3] S. P. Slinker, R. D. Taylor, and A. W. Ali. Electron energy deposition in atomic oxygen. *Journal of Applied Physics*, 63(1):1–10, jan 1988.