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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. In order to determine the partial pressures of the various species of residual gas in the gun chamber, each substantial peak was identified and fit with a Gaussian function of the form

$$f(x) = A \exp\left(-\frac{(x-b)^2}{2\sigma^2}\right) \tag{1}$$

where A is the height of the peak, b is the position (x-axis coordinate) of the center of the peak, and σ is the standard deviation. NOTE: The peak values must be divided by the correction factors listed here: https://www.mksinst.com/docs/ur/GaugeGasCorrection.aspx

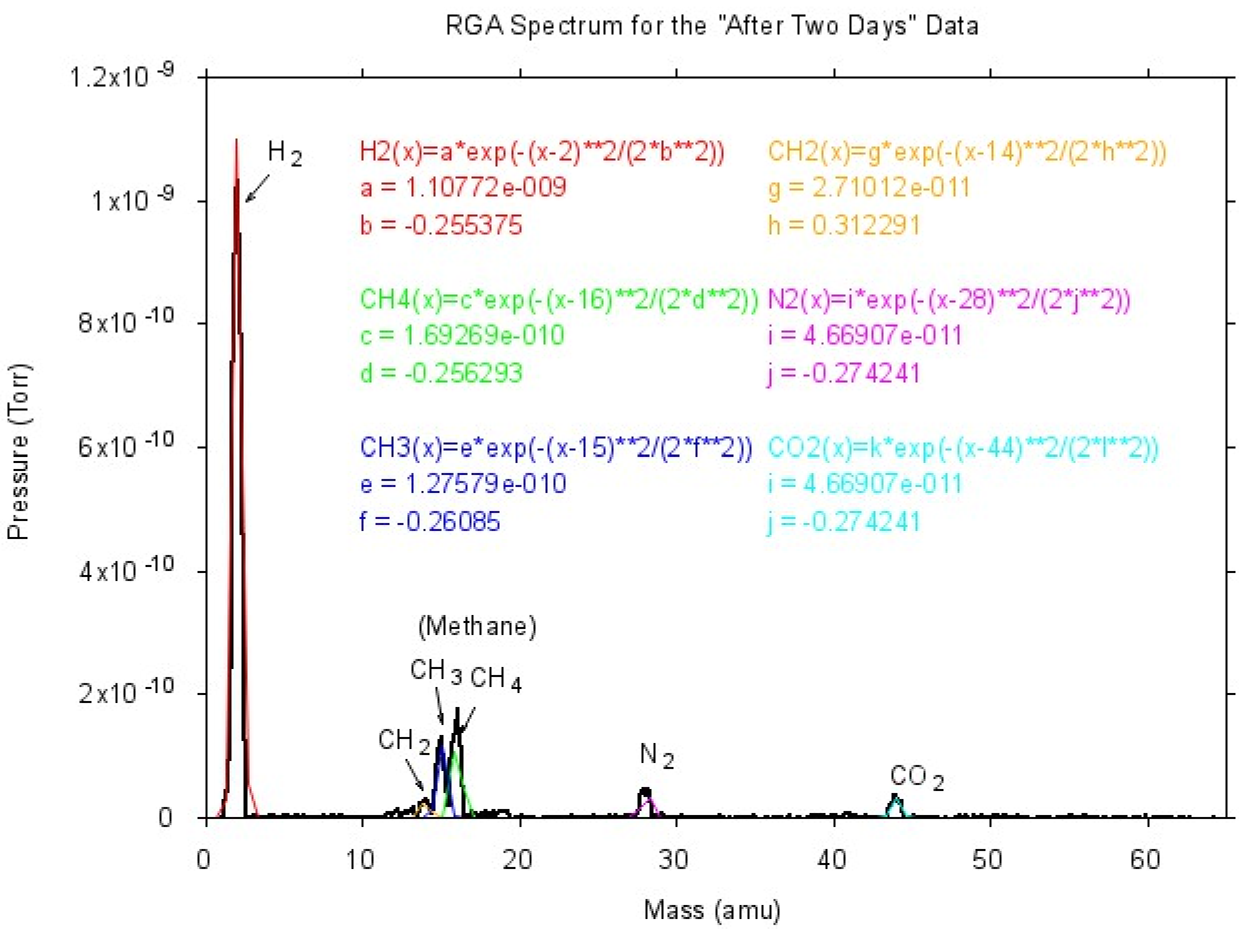

Figure 1: Analysis of the RGA spectrum for the "After 2 Days" data (before correction factor)

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]:

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

Numerically, this can be rewritten as:

$$\sigma_{i[\mathrm{m}^2]} = \frac{1.872 \times 10^{-24} A_1}{\beta^2} f(\beta) \left[\ln \left(7.515 \times 10^4 A_2 \beta^2 \gamma^2 \right) - \beta^2 \right] \tag{3}$$

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:

$$f(\beta) = \frac{I_i}{T_e} \left(\frac{T_e}{I_i} - 1 \right) = \frac{2I_i}{m_e c^2 \beta^2} \left(\frac{m_e c^2 \beta^2}{2I_i} - 1 \right) \tag{4}$$

$$A_1 = M^2 \tag{5}$$

$$A_2 = \frac{e^{\frac{C}{M^2}}}{7.515 \times 10^4} \tag{6}$$

where C and M^2 are parameters given by Rieke and Prepejchal [2]. For H_2, CH_4, 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 the main 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:

$$\begin{aligned}
T_e &= (\gamma_e - 1) m_e c^2 = 200\text{keV} \\
m_e c^2 &= 511\text{keV} \\
\gamma_e &= 1 + \frac{T_e}{m_e c^2} = 1.39 \\
\beta_e &= \sqrt{1 - \frac{1}{\gamma_e^2}} = 0.695 \left(= 2.08 \times 10^8 \frac{\text{m}}{\text{s}} \right) \\
f(\beta_e) &= \frac{I_i}{T_e} \left(\frac{T_e}{I_i} - 1 \right) \approx 1 \\
\sigma_i &= \frac{1.872 \times 10^{-24} A_1}{\beta_e^2} f(\beta_e) \left[\ln \left(7.515 \times 10^4 A_2 \beta_e^2 \gamma_e^2 \right) - \beta_e^2 \right] \\
&\approx 2.99 \times 10^{-23} \text{m}^2
\end{aligned}$$

3 Ionization Rate

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

$$\frac{dn}{dt} = n_b n_g \sigma_i v = n_b n_g \sigma_i \beta_e c \tag{7}$$

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:

$$n_0 = \frac{p_0}{k_B T_0} \approx 2.687 \times 10^{25}\text{m}^{-3} \tag{8}$$

Thus, for a given gas, its density is

$$n_g \left[\text{m}^{-3}\right] = \left(3.54 \times 10^{22}\right) p\,(\text{torr}) \tag{9}$$

The partial pressures are calculated from the Gaussian fit functions in Figure (1), which are of the form of equation (1), using the Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}} \tag{10}$$

$$\int_{-\infty}^{\infty} A e^{-\frac{(x+b)^2}{2\sigma^2}} dx = A\sqrt{2\pi\sigma^2}$$

These partial pressures then need to be corrected using correction factors that adjust the pressures of the gas species relative to nitrogen N_2 (see link in Section 1). The correction factor for each parent ion is assumed to be the same for each ion in its class (as in the case of CH_4, CH_3, and CH_2). Assuming an extractor gauge pressure of 2×10^{-12}torr, we can normalize these partial pressures by a correction factor α that is equal to the sum of the corrected partial pressures divided by the extractor gauge pressure. Each partial pressure is then multiplied by α so that the sum of the partial pressures is 2×10^{-12}torr. In this case, $\alpha \approx 2.87 \times 10^{-3}$. From the normalized partial pressures, the number densities for each of the gases are calculated using eq. (9) and the production rate is calculated using equation (7). The results for each gas species in the RGA spectrum is shown in Tables 2 and 3 below.

Gas species	Uncorrected Pressure (torr)	Correction factor	Corrected Pressure (torr)	Normalized Pressure (torr)
H_2	7.09085×10^{-10}	0.46	3.26×10^{-10}	9.28×10^{-13}
CH_4	1.08744×10^{-10}	1.40	1.52×10^{-10}	4.33×10^{-13}
CH_3	8.34180×10^{-11}	1.40	1.17×10^{-10}	3.33×10^{-13}
CH_2	2.12148×10^{-11}	1.40	2.97×10^{-11}	8.45×10^{-14}
N_2	3.20961×10^{-11}	1.00	3.21×10^{-11}	9.14×10^{-14}
CO_2	3.20961×10^{-11}	1.42	4.56×10^{-11}	1.30×10^{-13}

Table 2: Data for the uncorrected, corrected, and normalized partial pressures of each gas species.

Gas species	Gas Density n_g $\left(\text{molecules/m}^3\right)$	Ionization Cross Section σ_i $\left(\text{m}^2\right)$	Ion Production Rate (ions/s)
H_2	3.29×10^{10}	2.99×10^{-23}	4.06×10^{17}
CH_4	1.53×10^{10}	1.53×10^{-22}	9.66×10^{17}
CH_3	1.18×10^{10}	8.00×10^{-23} *	3.89×10^{17}
CH_2	2.99×10^{9}	9.00×10^{-23}*	1.11×10^{17}
N_2	3.24×10^{9}	1.27×10^{-22}	1.70×10^{17}
CO_2	4.60×10^{9}	2.04×10^{-22}	3.87×10^{17}

Table 3: Data for the gas (number) density, ionization cross section, and ion production rate for each gas species assuming a 200keV beam. *Denotes values from NIST using the Binary-Encounter-Bethe (BEB) model here https://physics.nist.gov/PhysRefData/Ionization/intro.html

As an example calculation for H_2, the uncorrected partial pressure using equation (10) with is $p_{H_2,uncorr} = 7.09085 \times 10^{-10}$torr. The correction factor for H_2 is 0.46, so the corrected partial pressure is $p_{H_2,corr} = 3.26 \times 10^{-10}$torr. Multiplying this by α yields the normalized pressure $p_{H_2,norm} = 9.28 \times 10^{-13}$torr. From equation (9), the density of the H_2 gas is $n_{H_2} = 3.29 \times 10^{10}\mathrm{m}^{-3}$. The ionization cross section for H_2 is derived from equation (3), as shown in the numerical example in Section 2, and is $\sigma_{H_2} = 2.99 \times 10^{-23}\mathrm{m}^2$. Assuming we have a 200keV, 1mA uniform, cylindrical electron beam with an average transverse size of 1mm, then $T_e = 200$keV, $I = 1$mA, and $n_b \approx 1.98 \times 10^{21}\mathrm{m}^{-3}$. Then for H_2, the ionization rate is:

$$\begin{aligned}
\frac{dn_{H_2}}{dt} &= n_{H_2} n_b \sigma_{H_2} \beta_e c \\
&= \left(3.29 \times 10^{10}\mathrm{m}^{-3}\right)\left(1.98 \times 10^{21}\mathrm{m}^{-3}\right)\left(2.99 \times 10^{-23}\mathrm{m}^2\right)(0.695)\left(2.998 \times 10^8 \frac{\mathrm{m}}{\mathrm{s}}\right) \\
&\approx 4.06 \times 10^{17}\mathrm{m}^{-3}\,\mathrm{s}^{-1}
\end{aligned}$$

4 Ionization Cross Section vs. T_e

Starting from equation (3),

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

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:

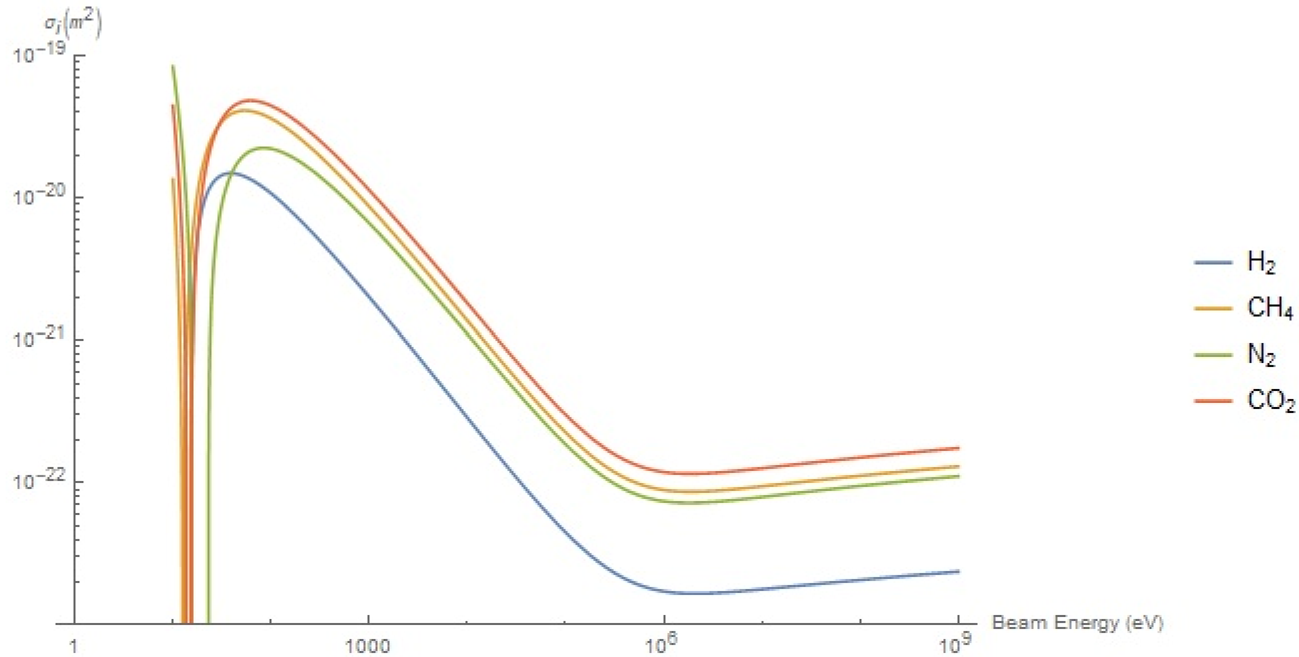

Figure 2: Plot of the ionization cross section σ_i vs. electron kinetic energy T_e

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.