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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

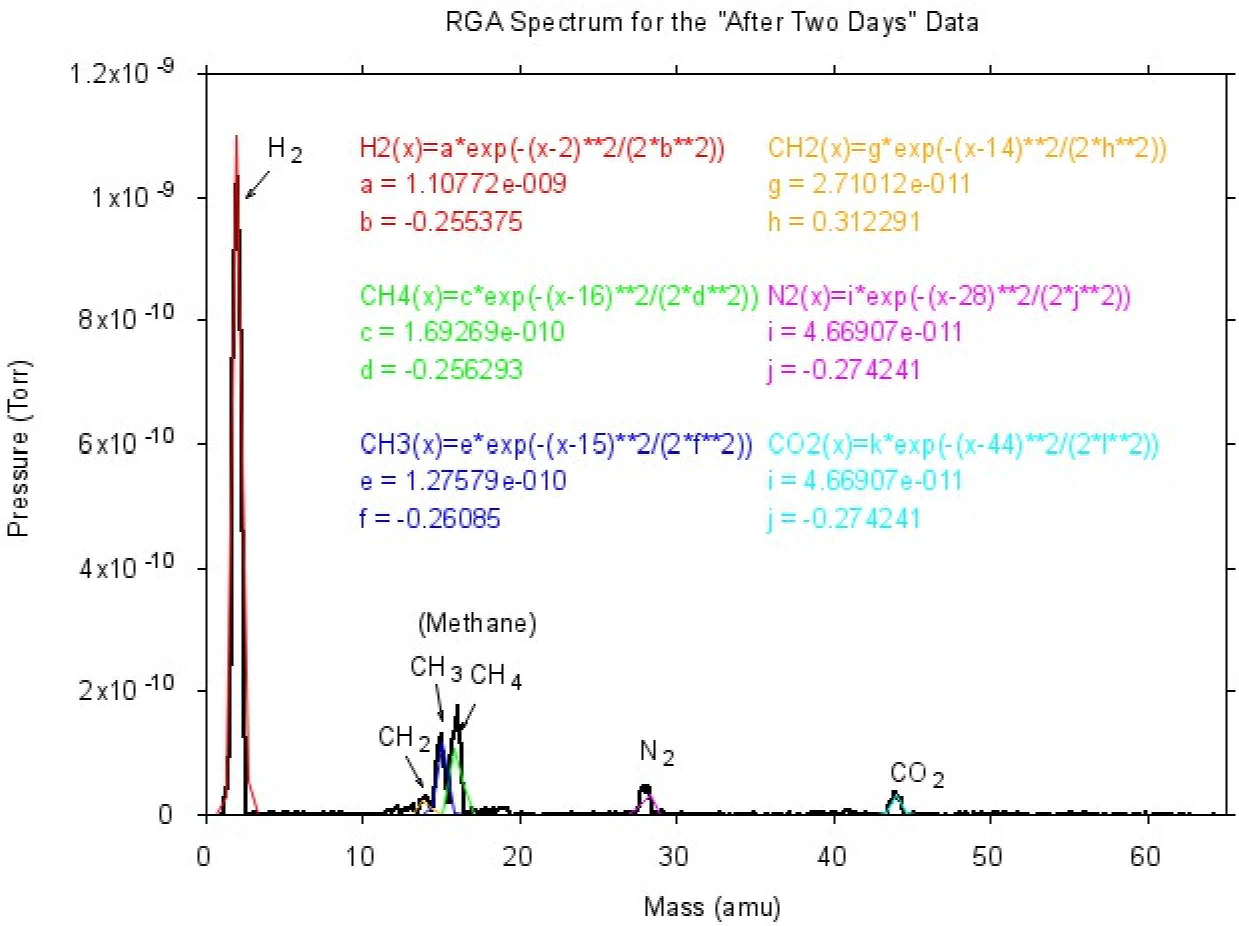

Figure 1: Analysis of the RGA spectrum for the "After 2 Days" data (before correction factor)

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:

$$\sigma_{i[\mathrm{m}^2]} = \frac{1.872\times10^{-24}A_1}{\beta^2} f(\beta)\left[\ln\left(7.515\times10^4 A_2\beta^2\gamma^2\right)-\beta^2\right] \tag{2}$$

In these two equations, $a_0 = 5.29\times10^{-11}$m is the Bohr radius, $I_R = 13.6$eV is the Rydberg energy, m_ec^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:

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

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

$$A_2 = \frac{e^{\frac{C}{M^2}}}{7.515\times10^4} \tag{5}$$

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, $m_ec^2 = 511$keV,

$$\begin{aligned}
T_e &= (\gamma_e - 1)\, m_ec^2 = 200\text{keV} \\
m_ec^2 &= 511\text{keV} \\
\gamma_e &= 1 + \frac{T_e}{m_ec^2} = 1.39 \\
\beta_e &= \sqrt{1-\frac{1}{\gamma_e^2}} = 0.695 \left(= 2.08\times10^8\,\frac{\text{m}}{\text{s}}\right) \\
f(\beta_e) &= \frac{I_i}{T_e}\left(\frac{T_e}{I_i}-1\right) \approx 1 \\
\sigma_i &= \frac{1.872\times10^{-24}A_1}{\beta_e^2} f(\beta_e)\left[\ln\left(7.515\times10^4 A_2\beta_e^2\gamma_e^2\right)-\beta_e^2\right] \\
&\approx 2.994\times10^{-23}\text{m}^2
\end{aligned}$$

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

$$\frac{dn}{dt} = n_bn_g\sigma_iv = n_bn_g\sigma_i\beta_ec \tag{6}$$

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

$$n_0 = \frac{p_0}{k_BT_0} \approx 2.687\times10^{25}\text{m}^{-3} \tag{7}$$

Thus, for a given gas, its density is

$$n_g\left[\mathrm{m}^{-3}\right]=\left(3.54\times10^{22}\right)p\,(\mathrm{torr})$$

For H_2, $p\,(\mathrm{torr})$ can be read off from Figure 1. In this case, $p_{H_2}=1.11\times10^{-9}$torr with a correction factor of 0.46 for H_2, so $n_{H_2}=8.54\times10^{13}\mathrm{m}^{-3}$. Knowing the electron density in the beam, n_b, one can calculate the ionization rate $\frac{dn}{dt}$.

3 Ionization Cross Section vs. T_e

Starting from equation (2),

$$\sigma_i\left[\mathrm{m}^2\right]=\frac{1.872\times10^{-24}A_1}{\beta^2}\frac{I_i}{T_e}\left(\frac{T_e}{I_i}-1\right)\left[\ln\left(7.515\times10^4A_2\beta^2\gamma^2\right)-\beta^2\right]$$

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

$$T_e=(\gamma-1)\,m_ec^2$$
$$\gamma=1+\frac{T_e}{m_ec^2}$$
$$\frac{1}{\sqrt{1-\beta^2}}=1+\frac{T_e}{m_ec^2}$$
$$1-\beta^2=\left(\frac{1}{1+\frac{T_e}{m_ec^2}}\right)^2=\left(\frac{m_ec^2}{m_ec^2+T_e}\right)^2$$
$$\beta^2=1-\left(\frac{m_ec^2}{m_ec^2+T_e}\right)^2$$

Thus,

$$\sigma_i=\frac{1.872\times10^{-24}A_1}{1-\left(\frac{m_ec^2}{m_ec^2+T_e}\right)^2}\frac{I_i}{T_e}\left(\frac{T_e}{I_i}-1\right)\left[\ln\left(7.515\times10^4A_2\left(1-\left(\frac{m_ec^2}{m_ec^2+T_e}\right)^2\right)\left(1+\frac{T_e}{m_ec^2}\right)\right)-\left(1-\left(\frac{m_ec^2}{m_ec^2+T_e}\right)^2\right)\right]$$

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

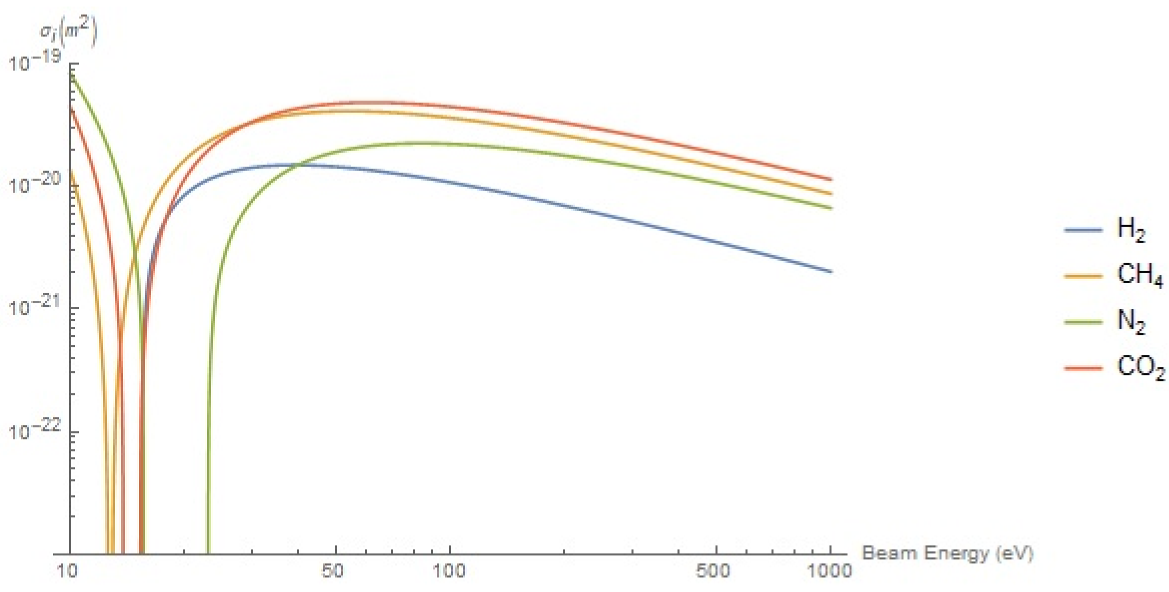

Figure 2: Plot of the ionization cross section σ_i vs. electron kinetic energy T_e

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.