

Supporting Information: Electrical stability and performance of a Nitrogen-Oxygen atmospheric pressure gliding arc plasma

Filippo Manaigo,^{*,†,‡} Omid Samadi Bahnamiri,[†] Abhyuday Chatterjee,[†] Adriano Panepinto,[¶] Arnaud Krumpmann,[¶] Matthieu Michiels,[¶] Annemie Bogaerts,[‡] and Rony Snyders^{†,¶}

[†]*Research Group ChIPS, Department of Chemistry, University of Mons, Av. Nicolas Copernic 3, 7000 Mons, Belgium*

[‡]*Research Group PLASMANT, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium*

[¶]*Materia Nova Research Center, Parc Initialis, 7000 Mons, Belgium*

E-mail: filippo.manaigo@umons.ac.be

Contents

1 FTIR Data Analysis	3
----------------------	---

List of Figures

1 FTIR spectra acquired between 1000 and 3500 cm^{-1} for $\langle I \rangle$ equal to 120 mA. The absorption bands at 1876 cm^{-1} and 2916 cm^{-1} were used for NO and NO ₂ respectively	3
---	---

1 FTIR Data Analysis

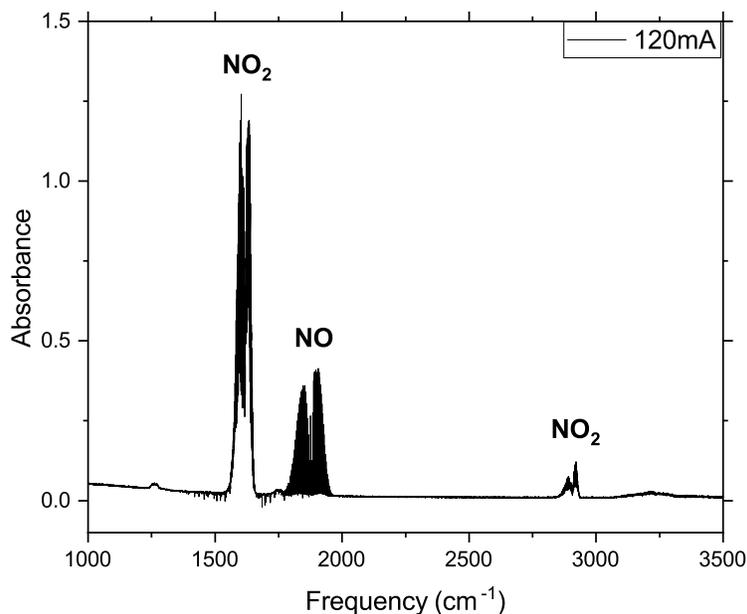


Figure 1: FTIR spectra acquired between 1000 and 3500 cm^{-1} for $\langle I \rangle$ equal to 120 mA. The absorption bands at 1876 cm^{-1} and 2916 cm^{-1} were used for NO and NO₂ respectively

The IR beam is attenuated after passing through the gas contained in the gas cell. The intensity of the attenuated beam can be described using the Beer-Lambert absorption law, assuming a homogeneous density distribution.^{1,2} Finally, the absorbance, defined as the logarithm of the ratio of the initial and the detected beam intensities, is calculated.

Figure 1 shows an example of an absorption spectrum in this work. The only species observed by FTIR absorption spectroscopy are NO and NO₂, measured through their transitions with main band heads at 1876 cm^{-1} and at 2916 cm^{-1} , respectively. The NO₂ band located at 1617 cm^{-1} was not used due to its high absorbance. An absorbance above 1 corresponds to less than 10% of the incident photons with a specific wavelength reaching the detector. This is generally considered too low for the FTIR measurement to be consistent and for the linear dependency with the NO₂ concentration, described by the Beer-Lambert

law to be valid. The considered NO transition corresponds to the absorption due to the excitations from the ground state to the first vibrational level.³ The mentioned NO₂ transitions are, as well, excitation to low vibrational assignments from the ground state.⁴ Considering that there is no overlap between the spectra of the two species, their contribution to the total absorbance can be easily distinguished. The absorbance $A(\nu)$ of NO and NO₂ in the presence of plasma can be integrated and compared with the calibrated spectra in order to deduce their absolute densities using Beer-Lambert's law.

$$\begin{aligned} \int A(\nu) &= \int \sum_j n_j \sigma_j(\nu) d\nu = \sum_j n_j \int \sigma_j(\nu) d\nu \\ &= n_{NO} \int \sigma_{NO}(\nu) d\nu + n_{NO_2} \int \sigma_{NO_2}(\nu) d\nu \end{aligned} \quad (1)$$

Where, n_j and $\sigma_j(\nu)$ are the densities and the cross sections, respectively, for photon absorption as a function of the incident frequency of all the sampled species j . As NO and NO₂ are the only species probed by FTIR in the reactor, the equation is simplified in the last step. As a result of the fact that the integral of the cross sections is constant, the ratio between the absorbance of a plasma-generated gas mixture and the calibration gas set of measurements corresponds to their NO or NO₂ density ratio. In this work, part of the results is shown in terms of the NO_x yield, combining NO and NO₂ together according to the following equation:

$$\text{NO}_x \text{ Yield} = \frac{(n_{NO} + n_{NO_2})}{n_0} 100\% \quad (2)$$

where n_0 is the initial gas density. The statistical error associated with the absorbance value is determined by repeating measurements for the same experimental conditions and estimated to be of the order of 1% of the measured values.

References

- (1) Samadi Bahnamiri, O.; Verheyen, C.; Snyders, R.; Bogaerts, A.; Britun, N. Nitrogen fixation in pulsed microwave discharge studied by infrared absorption combined with modelling. *Plasma Sources Science and Technology* **2021**, *30*, 065007.
- (2) Engeln, R.; Klarenaar, B.; Guaitella, O. Foundations of optical diagnostics in low-temperature plasmas. *Plasma Sources Science and Technology* **2020**, *29*, 063001.
- (3) Goldman, A.; Brown, L. R.; Schoenfeld, W. G.; Spencer, M. N.; Chackerian, C.; Giver, L. P.; Dothe, H.; Rinsald, C. P.; Coudert, L. H.; Dana, V.; Mandin, J. Nitric Oxide Line Parameters: Review of 1996 Hitran Update and New Results. *J. Quant. Spectrosc. Radiat. Transfer* **1998**, *60*, 825–838.
- (4) Perrin, A.; Flaud, J. M.; Goldman, A.; Camy Peiret, C.; Lafferty, W. J.; Arcas, P.; Rinsald, C. P. NO₂ and SO₂ Line Parameters: 1996 Hitran Update and New Results. *J. Quant. Spectrosc. Radiat. Transfer* **1998**, *60*, 839–850.