PRECISION
Strategic Research Cluster

Use of “tuned” particle in cell simulations for absolute atomic oxygen number density determination using actinometry

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Introduction:

- **Actinometry** is a non-invasive optical technique that allows absolute atomic oxygen number density [O] to be measured in plasma provided certain conditions are met.
- **Problem:** Technique is sensitive to the accuracy of the Electron Energy Distribution Function (EEDF).
- **Maxwellian distribution** is often used for actinometry calculations but this is not appropriate in many cases.
- **This work:** We investigate use of **“**Tuned” Particle in Cell (PIC) simulation to generate more reliable EEDFs over a range of RF powers for a 100 mTorr oxygen/argon plasma. PIC simulations are tuned by adjusting input parameters until the PIC yields an electron density n_e that matches n_e values measured using a hairpin probe .
- **Two-photon Absorption Laser Induced Fluorescence (TALIF)** [O] is used as a benchmark to validate the [O] results obtained from actinometry with the EEDFs obtained from the tuned PIC simulations.

Actinometry:

- Comparison of the intensity of O emission lines at 884 nm with Ar emission at 750 nm obtained from a known concentration of Argon [Ar] within the plasma allows [O] to be determined.

[O] is calculated using the actinometry expression:

$$[\mathrm{O}] = \frac{\mathrm{I_O}}{\mathrm{I_{Ar}}}[\mathrm{Ar}]\frac{k_e^{Ar}}{k_e^{O}}\frac{1}{\gamma} - \frac{k_{de}^{O}}{k_e^{O}}[\mathrm{O_2}]$$

Note: The 844 nm emission line of O is chosen as previous works have found that it is less prone to dissociative excitation contributions which can make the actinometry technique unreliable [1].

where

$$\gamma = \frac{c_{(O)}\upsilon_{(O)}A_{ij}^{(O)}\left(k_q^{Ar}[O_2]+\sum_j A_{ij}^{Ar}\right)}{c_{(Ar)}\upsilon_{(Ar)}A_{ij}^{(Ar)}\left(k_q^{O}[O_2]+\sum_j A_{ij}^{O}\right)}$$

where k_e: Rate coefficient for excitation of upper level via electron collision.
I_o, I_{Ar}: Spectral intensities of O and Ar emission lines from the plasma.
γ: Constant that incorporates optical and geometric parameters such as solid angle, frequency of emitted light, transmission of optics etc. *provided* $[o_2]$ *remains constant*.

The determination of [O] depends strongly on the rate coefficients k_i - all other quantities in the expression essentially remain fixed for a given set of experimental conditions.

Rate constants and EEDF:

- Rate constant k_e is calculated using:

$$k_e = \int_0^{\infty} f(E)\sigma\sqrt{\frac{2E}{m_e}}\,dE$$

where $f(E)$: Normalized EEDF.
m_e: Electron mass.
σ: Electron collision cross section.
E: Electron energy.

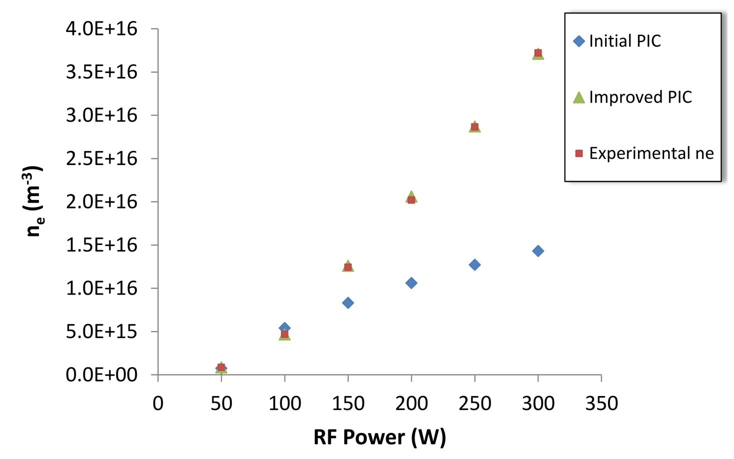
Expression shows the rate coefficients are sensitive to the form of the EEDF $f(E)$.

Improved accuracy of EEDF → improved accuracy of actinometry [O] results.

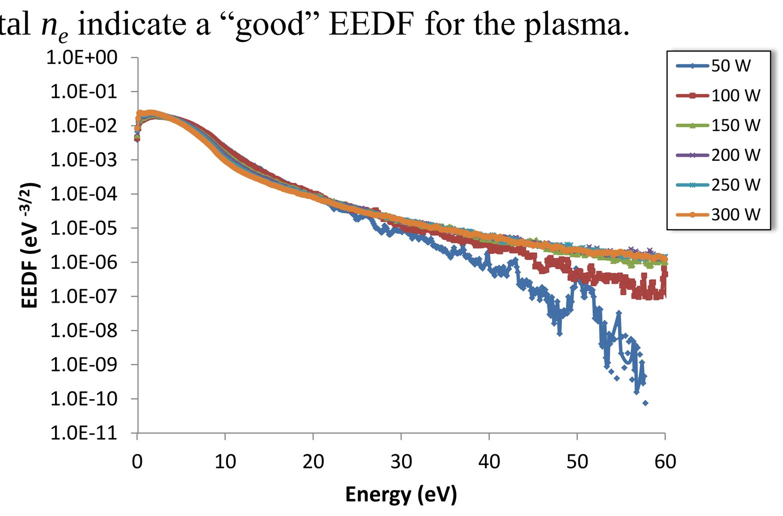
Particle In Cell (PIC) simulation:

- Fluid model approach that uses basic physics of particle interactions to arrive at the plasma conditions.
- Input variables to “tune” the simulation to the plasma are:
  (1) RF input voltage.
  (2) Secondary electron yield coefficient at walls.

- The simulation generates the EEDF, and electron density n_e for a given set of conditions.
- The calculated n_e from the code can be compared with a measured value of n_e obtained using a hairpin probe on the system to validate the simulation.
- Comparable values of the theoretical and experimental n_e indicate a “good” EEDF for the plasma.



(a) Graph of n_e from the initial PIC and final “tuned” PIC simulations compared with those measured with hairpin probe.



(b) Graph of EEDFs from “tuned” PIC code

References:

[1] H M Katsch, A Tewes, E Quandt, A Goehlich, T Kawetzki, H F Döbele, J. Appl. Phys. 88 (2000) 6232.
[2] N S Braithwaite, Pure and Appl. Chem. 62 (1990) 1721.
[3] J S Jeng, J Ding, J W Taylor, N Hershkowitz, Plasma Sources Sci. Technol. 3 (1994) 154.
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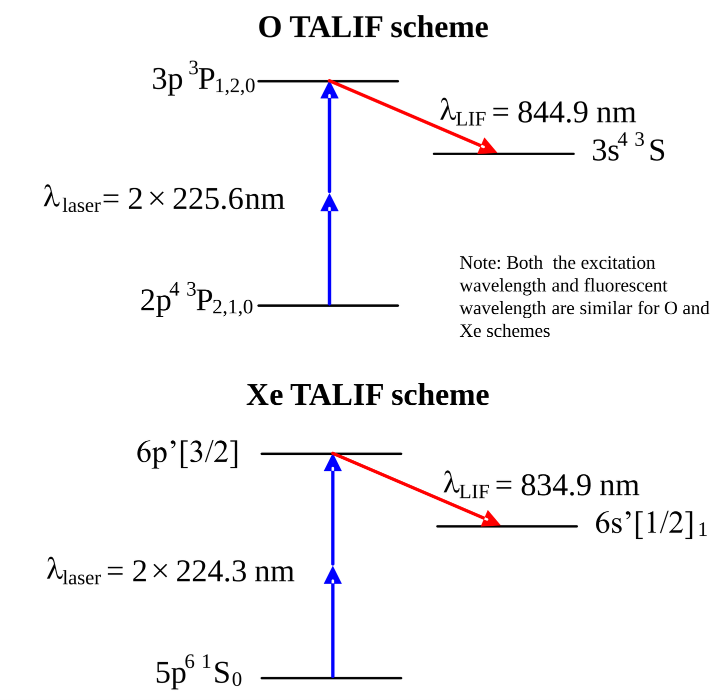
[6] M W Kielbauch, D B Graves, J Vac. Technol. A 32 (2003) 660.
[7] J Conway, S Kechkar, N O’Connor, C Gaman, MM Turner, S Daniels, Plasma Sources Sci. Technol. 22 (2013) 045004.

Two-photon Absorption Laser Induced Fluorescence (TALIF):

- **TALIF** allows [O] to be determined when calibrated with an appropriate Noble gas two-photon scheme such as that of Xenon given below.
- Excitation and fluorescent detection conditions must be similar for both O and Xe TALIF.
- The laser must operate at powers that ensure an unsaturated quadratic response from the detection system for both O and Xe.



- [O] is calculated using:

$$n_O = \chi\frac{S_O}{S_{Xe}}n_{Xe}$$

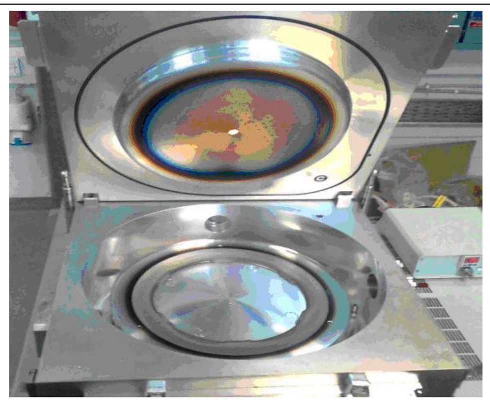
where: S_o, S_{Xe}: measured TALIF signals integrated w.r.t. time, fluorescent wavelength, excitation wavelength and normalised to the square of the laser pulse energy.

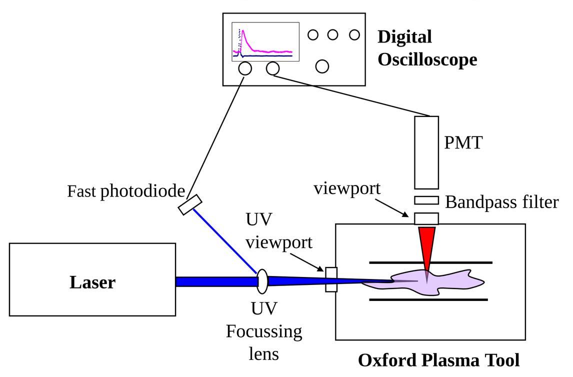
χ is a constant that takes account of the optical transmission of the system T_i and quantum efficiency of the detector η_i at the fluorescent wavelengths λ_i, the two-photon absorption cross sections σ_i and the effective branching ratios a_i.

$$\chi = \frac{T_{Xe}}{T_O}\frac{\eta_{Xe}}{\eta_O}\frac{\sigma_{Xe}^{(2)}}{\sigma_O^{(2)}}\frac{a_{21}^{Xe}}{a_{21}^{O}}\left(\frac{\lambda_{Xe}}{\lambda_O}\right)^2$$

Experiment:

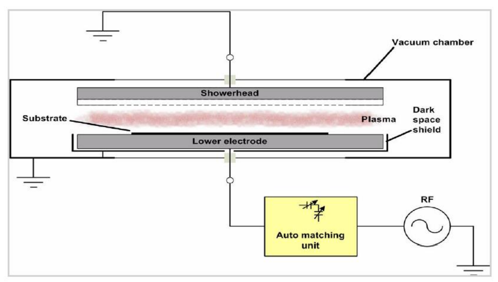
- Oxford instruments Plasmalab System 100 reactive ion etcher.
- Parallel plate capacitive asymmetric RF plasma system
- Wafer is placed on the lower powered electrode and gas feed through a showerhead designed into the upper ground electrode.
- A feedstock gas mixture comprising 96:4 % O_2:Ar at 100 mTorr was introduced into the chamber and RF power varied.
- TALIF and optical emission spectra were recorded at each power setting.





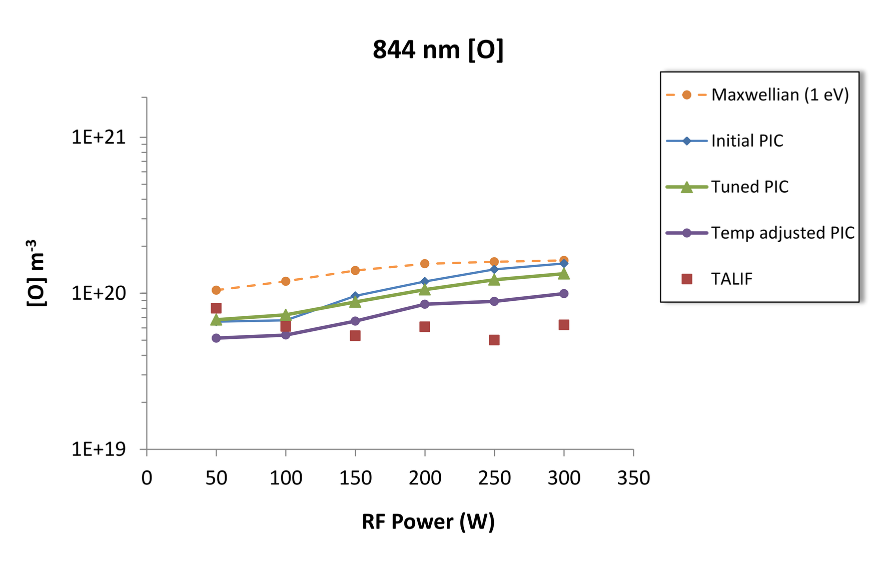
TALIF experiment:

Laser light at 226nm is focussed into chamber using UV optics. The resulting fluorescence at 844 nm is detected using a PM tube. An optical bandpass filter is used to attenuate the background light from the plasma so only the laser induced fluorescence reaches the detector.



Comparison of actinometry results obtained using PIC EEDF and Maxwellian EEDF with TALIF results for [O]:

- Absolute [O] number density was calculated using Maxwellian EEDF and PIC EEDF with actinometry.
- Results plotted along with TALIF data for comparison below.



- TALIF measurements show [O] ~ 6 x 10^{19} m^{-3} and decreases slightly with increasing RF power.
- Maxwellian EEDF gives worst agreement with TALIF [O].
- Optimized PIC EEDF where experimental and simulated n_e are matched give better agreement between actinometry and TALIF [O] result.
- Gas Temperature effects when included were found to further improve agreement.
- Actinometry indicates a slight increase in [O] with increasing RF power but TALIF shows a slight [O] decrease.

Discussion: - For full description of work presented in this poster see reference [7].

- An attempt to improve the EEDF used in actinometry [O] calculations is made where PIC simulations are tuned to the electron density measured in a 100 mTorr O_2/Ar Plasma at various RF powers. The presumption is that the resulting EEDF will more accurately reflect the true EEDF in the plasma.
- [O] results obtained using the actinometry technique incorporating the resulting EEDF are compared to those measured using TALIF which is known to be reliable technique.
- Use of a Maxwellian EEDF gave the poorest agreement between TALIF [O] and actinometry [O].
- Initial PIC simulation run using the RF voltage input recorded from the plasma tool for the various settings yielded n_e values that differed from experimental values for n_e measured with a hairpin probe. However, the corresponding actinometry [O] values still gave better agreement with TALIF [O] than a Maxwellian EEDF
- The PIC was tuned by varying the input voltage and to a lesser extent the secondary electron yield from the walls till the resulting n_e agreed with the experimental values. The [O] obtained from actinometry using this EEDF gave an improved agreement with TALIF results.
- The gas temperature was measured with a thermocouple and was found to increase as RF power increased. This affects species number densities and quenching in the plasma. Inclusion of temperature effects in actinometry calculations which used the optimized EEDF from the tuned PIC gave the best agreement between actinometry [O] and TALIF [O].

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