ERNST-MORITZ-ARNDT UNIVERSITY OF GREIFSWALD

MASTER THESIS

Kinetic effects in RF discharges

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"Without encroaching upon grounds appertaining to the theologian and the philosopher, the domain of natural sciences is surely broad enough to satisfy the wildest ambition of its devotees. [...] The work may be hard, and the discipline severe; but the interest never fails, and great is the privilege of achievement."

— John William Strutt, 3rd Baron Rayleigh, 1884 in: Address to the British Association in Montreal

Declaration of Authorship

I hereby certify that this thesis has been composed by me and is based on my own work, unless stated otherwise. No other person's work has been used without due acknowledgement in this thesis. All references and verbatim extracts have been quoted, and iall sources of information, including graphs and data sets, have been specifically acknowledged.

Signature of author

Signature of author Greifswald; July 19, 2017

Contents

| 0 | Abs | stract | 1 |
|---|------------------|--|----|
| 1 | Phy | vsical properties of low temperature RF plasma | 3 |
| | 1.1 | Plasma physics | 3 |
| | | 1.1.1 Capacitively coupled radio frequency plasma | 3 |
| | | 1.1.2 Sheath physics and wall interaction | 6 |
| | | 1.1.3 Self bias voltage | 6 |
| | | 1.1.4 Dielectric displacement current | 6 |
| | 1.2 | Negative ion physics | 6 |
| | | 1.2.1 Anion creation and distribution | 6 |
| | | 1.2.2 Dynamics and collisions | 6 |
| | 1.3 | Particle-In-Cell simulations with Monte Carlo-Colissions | 6 |
| | | 1.3.1 Principles | 6 |
| | | 1.3.2 2d3v PIC | 6 |
| | | 1.3.3 Monte Carlo-Collisions | 6 |
| 2 | Vali | idation of Simulation by 1d comparison | 7 |
| _ | 2.1 | Axial density profiles | 7 |
| | 2.2 | Velocity and energy distributions | 7 |
| | 2.3 | Transition to 2d simulation | 7 |
| 3 | Sim | ulation of capacitively coupled rf discharges | 9 |
| | 3.1 | Experimental setup | 9 |
| | 3.2 | Secondary ion emission | 9 |
| | 3.3 | Anion energy distributions in oxygen | 9 |
| 4 | Eni | logue | 11 |
| _ | $\frac{-1}{4.1}$ | Local electrostratic field solver | 11 |
| | 4.2 | Diagnostics of current and charge | 11 |
| | 4.3 | Field calculation | 11 |
| | 4.4 | Comparison with Poisson-based solvers | 11 |
| 5 | Cor | nclusion | 13 |

Physical Quantities

| Quantity | Unit | Symbol | Dimension | Value |
|---------------------|-----------------|---------------|--------------------------|---|
| Speed of Light | $\frac{m}{s}$ | c_0 | | $2,997 \cdot 10^8$ |
| Vacuum permittivity | $\frac{F}{m}$ | $arepsilon_0$ | $s^4 A^2 m^{-3} kg^{-1}$ | $8,854 \cdot 10^{-12}$ |
| Boltzmann constant | $\frac{eV}{K}$ | $k_{ m B}$ | $\rm JK^{-1}$ | $8,\!617\cdot 10^{-23}$ |
| particle density | ${\rm cm}^{-3}$ | $n_{ m j}$ | m^{-3} | |
| kinetic temperature | eV | $T_{ m j}$ | K | |
| elementary charge | \mathbf{C} | e | As | $1,902 \cdot 10^{-19}$ |
| particle mass | kg | $m_{ m j}$ | | electron: $9,109 \cdot 10^{-31}$ ion: $5,3110^{-26}$ anion: $5,14310^{-26}$ |

Abstract

The Thesis Abstract is written here and usually kept to just this page. The page is kept centered vertically so it can expand into the blank space above the title too.

Physical properties of low temperature RF plasma

In this first chapter I will provide the necessary physical background for this work about the numerical simulation of low temperature capacitively coupled radio frequency plasma. Here both the mathematical basics and method for the simulation, as well as the most important aspects about the plasma properties will be explained.

1.1 Plasma physics

1.1.1 Capacitively coupled radio frequency plasma

The experiment where after the conducted simulation is modelled after resembles a capacitively coupled radio frequency, low temperature plasma at low pressures of oxygen.

Here, I will refer to a plasma as an globally quasi-neutral gas, consisting of freely moving charges — e.g. electrons, anions and kations — and neutral gas particles. The ratio between charged and neutral species defines the *degree of ionization*, which in this case is very low. The term of global neutrality emphasizes the purpose for different length scales inside the gas itself. Here, the associated condition $n_e = n_i$ only is valid for areas larger than the so called *Debye sphere*. Inside this ball with a radius of λ_D , the *Debye length*, the afore-mentioned neutrality is not satisfied. A selection of the most important and basic physical properties and attributes have been compiled in table 1.1.

The creation of a plasma is accomplished by 2 parallel metal plates, the electrodes, where on at least one an alternating current at radio frequency is applied — this kind of experimental setup is among the most common, thus being used for basic but also in-depth studies of such discharges. Here, a rf signal at exactly 13,56 MHz with an amplitude between 100–1000 V will be used. This corresponds to a wavelength of 22,11 m for the external excitation. Within the scope of this work I will omit external magnetic fields.

That said, a multitude of electric setups are possible, such as coated or grounded electrodes. Therefore, different regimes of operation ensue. For example, differently driven or shaped metal plates heavily influence the charge creation process inside the plasma. In summary, the electrodes, neutral gas and electric layout resemble a dielectric hindered plate capacitor. This simplification can be used to access important physical properties, such as an additional voltage offset on one of the electrodes or charge currents at such. A basic scheme of an asymmetric rf discharge can be seen in ??.

In the case of different electrode sizes, as seen in the afore-mentioned scheme, the potential inside the spatially restricted area between wall — this can be also a grounded metal wall aside the electrodes — and discharge can change drastically. This additional direct current offset is called *self-bias* (see ??). A dielectric displacement current between plasma sheath and volume accomodates as a result of the different time scales of particle movement. Especially, self-bias and displacement current play a key role in the following investigations, as a capacitive coupling between electrodes and power supply is difficult to model into a numerical kinetic simulation.

| quantity | equation | relevance |
|------------------------------------|--|---|
| Debye length | $\lambda_{\mathrm{D,j}}^2 = rac{arepsilon_0 k_{\mathrm{B}} T_{\mathrm{j}}}{n_{\mathrm{j}} e^2}$ $\lambda_{\mathrm{D}}^2 = \left(\lambda_{\mathrm{D,e}}^{-2} + \lambda_{\mathrm{D,i}}^{-2} ight)^{-1}$ | distance around a charge, at which quasi-neutrality is satisfied, $\lambda_{\rm D}$ is the combined screening length from individual species |
| plasma parameter | $N_{\rm D} = n \frac{4}{3} \pi \lambda_{\rm D}^3$ | number of particles inside Debye sphere, if $N_{\rm D}\gg 1$ an ionized gas is considered a plasma (degree of ionization) |
| plasma frequency | $\omega_{\mathrm{p,j}}^2 = \frac{n_{\mathrm{j}}e^2}{\varepsilon_0 m_{\mathrm{j}}} = \frac{v_{\mathrm{th,j}}}{\lambda_{\mathrm{D,j}}} = \frac{1}{\tau_{\mathrm{j}}}$ | upper limit for interaction with fields/forces or exter- nal excitations inverse screen- ing time |
| thermal velocity | $v_{ m th,j}^2=rac{k_{ m B}T_{ m j}}{m_{ m j}}$ | mean velocity from kinetic theory of gases |
| coulomb logarithm | $\ln{(\Lambda)}$ $\Lambda = rac{b_{ m max}}{b_{ m min}} = \lambda_{ m D} \cdot rac{4\piarepsilon_0 \mu v_{ m th}^2}{e^2}$ | dimensionless scale for transport processes inside discharge fraction of probability for a cumulative 90° scattering by many small pertubation collisions and a single right angle scattering |
| collision frequency | $\nu_{0,j} = \frac{e^4 n_j \ln(\Lambda)}{8\sqrt{2m_j} \pi \varepsilon_0 (k_B T_j)^{3/2}}$ | two body coulomb collision frequency inside species j |
| particle distance & mean free path | $\overline{b} = rac{\hbar}{m_{ m j}v_{ m th,j}}$ $s_{ m mfp,j} = rac{v_{ m th,j}}{ u_{ m j,k}}$ | mean inter particle distance for species j free flight between subsequent collisions of species j and k with collision frequency $\nu_{j,k}$ |
| Debye-Hückel potential | $\Phi = \frac{Q}{4\pi\varepsilon \vec{r} }e^{-\frac{ \vec{r} }{\lambda_{\rm D}}}$ | electrostatic potential of charge particle Q at distance $ \vec{r} $ equal to coulomb interaction with additional shielding by charged particles inside debye sphere |

Table 1.1: Selection of physical properties of a low temperature ccrf discharge. The index j denotes the species, e.g. electrons, ions etc.

- 1.1.2 Sheath physics and wall interaction
- 1.1.3 Self bias voltage
- 1.1.4 Dielectric displacement current
- 1.2 Negative ion physics
- 1.2.1 Anion creation and distribution
- 1.2.2 Dynamics and collisions
- 1.3 Particle-In-Cell simulations with Monte Carlo-Colissions
- 1.3.1 Principles
- 1.3.2 2d3v PIC
- 1.3.3 Monte Carlo-Collisions

Validation of Simulation by 1d comparison

- 2.1 Axial density profiles
- 2.2 Velocity and energy distributions
- 2.3 Transition to 2d simulation

Simulation of capacitively coupled rf discharges

- 3.1 Experimental setup
- 3.2 Secondary ion emission
- 3.3 Anion energy distributions in oxygen

Epilogue

- 4.1 Local electrostratic field solver
- 4.2 Diagnostics of current and charge
- 4.3 Field calculation
- 4.4 Comparison with Poisson-based solvers

Conclusion