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MASTER

EUV spectroscopy of hydrogen plasmas

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EUV spectroscopy of hydrogen plasmas

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April 2009 EPG 09-02

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Abstract

Claims have been made that a discharge containing hydrogen produces previously unknown radiation in the extreme ultraviolet (EUV) range (10-70 nm). We try to verify these experimental results. For this a setup has been built with a vacuum system that consists of a plasma source, an EUV spectrometer and a detector.

We used two different plasma sources: a microwave plasma and a pulsed plasma. The microwave plasma is made with an Evenson cavity, which produces a continuous discharge. We used various gas mixtures of hydrogen, helium and argon. With the pulsed plasma source a discharge of about 400 ns is produced between a grounded anode and a cathode at –13 kV. The plasma is a hollow cathode triggered discharge, but to get better control we triggered the discharge with a pulsed electron beam aimed at the anode.

Light emitted by the plasma is analyzed with a grazing incidence EUV spectrometer with a Rowland circle of 2.2 m. For the detection of EUV photons we used a Channel Electron Multiplier (CEM). The setup has an instrumental profile with a measured FWHM of 8 pm, which is in agreement with the theoretical predictions. The wavelength range is 2-113 nm, and the central wavelength of a peak is calibrated to within 10 pm. The sensitivity of the spectrometer in combination with the CEM is good enough to see nearly all known emission lines in a microwave plasma of helium, hydrogen and argon. For spectroscopy in the visible wavelength range we used a Double Echelle Monochromator for high resolution spectra, and a small Czerny-Turner type spectrometer for full range measurements.

In a microwave plasma with He/H$_2$ (98/2%) we measured a broad feature between 62.7 and 63.4 nm. The feature only appears in mixtures with a low fraction of H$_2$. The feature is reported earlier by Mills et al.

In a pulsed H$_2$ plasma we measured a continuum between 23 and 30 nm. Also this continuum is reported by Mills et al. By counting the pulses from the CEM time resolved, it is possible to distinguish between pulses that are produced during the discharge and in the afterglow. We found that the continuum is mainly produced during the discharge. However the photon rate during the discharge exceeds the maximum count rate of the counting system, so the system is saturated.

In a pulsed He plasma we measured the afterglow of emission lines of He and He$^+$. The afterglow of He$^+$ lines lasts relatively long (20 µs), while the He lines have almost no afterglow.
The work presented in this thesis would never have been possible without the effort of many people; I will name just a few.

First of all I would like to thank my supervisors Gerrit Kroesen, Sander Nijdam and Eddie van Veldhuizen for their guidance and helpful discussions. Also Benjamin de Maat for being a very nice roommate, and (together with Sander) for introducing me into the world of Chinese food. I thank Evert Ridderhof for his technical support and his persuasion for visiting borrels, Ruud Wijtvliet for the preparations he did for my project, and also Ruud de Regt and Alexis Leray for their work on the project. I also had a great time on the trips to Washington and Princeton, and to several other conferences. I would like to thank the people from Blacklight Power Inc. for their interesting discussions, especially Ying Lu, who visited us for three weeks to help us with the pulsed source. Furthermore I thank the whole group EPG for the nice chats and countless times vlaai during the coffee break.

If would also like to thank my parents, who have supported me all my life and never doubted me.

And finally, I would like to thank my girlfriend Marinka Knops, for her love and support. I need her more than she might realize.

Bram van Gessel
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Chapter 1

Introduction

In recent years the American scientist Dr. Randell Mills and his company Blacklight Power Inc. have published results from experiments on plasmas containing hydrogen. These results triggered a discussion in the scientific world. The reason for this is twofold. The first reason is scientific curiosity. The experimental results are new, and finding an explanation proved to be not straightforward. Explaining the results could give interesting new insight in the involved plasma physics. The second reason is the explanation that Mills presents for his results, which is highly controversial. Mills propagates the idea of a new type of reaction with hydrogen, and this caused a great deal of controversy in the scientific world.

Of these two reasons we want to confine ourselves to the first, scientific curiosity, and leave the latter to the theoretical physicists. We have given ourselves the difficult task of redoing the experiments of Mills, without getting caught in the crossfire of the heated theoretical discussion.

1.1 Experimental status

In this thesis we will only discuss the results of Mills et al. that involve plasma physics. Mills claims that an exothermic reaction, which he calls the Blacklight process, can take place in a plasma with hydrogen and certain additions. These additions include gasses like helium or argon, and solids like strontium. The experiments Mills et al. did with these plasmas mainly involve three types: calorimetry, measurements of line broadening, and extreme ultraviolet (EUV) spectroscopy. In the introductory chapter we will discuss these three types of experiments. The rest of this thesis will be about EUV spectroscopy.

1.1.1 Calorimetry

In calorimetric experiments all the ingoing and outgoing energy fluxes of a plasma are measured. This way any energy that is produced by the plasma can be mea-
Mills et al. reported excess energy in different types of hydrogen plasmas, using different calorimetric techniques. These include optical calorimetry on glow discharge plasmas [1], calvet calorimetry on hollow cathode discharge plasmas [2] and water bath calorimetry on microwave plasmas and hollow cathode discharge plasmas [1, 3].

Experimentally these experiments can be difficult to perform accurately, due to all kinds of losses in almost all systems. Especially optical calorimetry is known to be very inaccurate. The results of Mills are criticized by Phelps [4]. His main point of criticism is the inaccurate measurement of the power inputs to the plasma, especially for microwave plasmas.

Sofar, there has been no independent confirmation of experimental results that show excess energy. At Eindhoven University of Technology experiments are done with a specially designed calorimeter [5]. The plasma which is used is a DC glow discharge with a mixture of Ar/H₂ and Sr. No excess energy is measured, although it must be said that the Sr was oxidized, which could have been a reason for the experiment to fail.

The theory and experimental results of calorimetry are discussed in detail in the Master’s thesis of Benjamin de Maat [5].

### 1.1.2 Extreme line broadening

It has been proposed that in plasmas containing hydrogen, under certain conditions, the hydrogen has a very high temperature. This high temperature causes a
1.1 Experimental status

Doppler broadening of emission lines of hydrogen. Visible spectroscopy is used to verify this. The emission lines H$_\alpha$ (656.5 nm) and H$_\beta$ (486.3 nm) are the most suited for measurements of the line width. As an example a result of De Maat in a DC glow discharge is shown in figure 1.1. It can be seen that the H$_\alpha$ line is broadened compared to the narrow Sr line. The width that is attributed to Doppler broadening suggests that the hydrogen has a temperature of 23.3 eV (or $2.7 \cdot 10^5$ K). This value is unusually high.

Extreme line broadening suggesting a high temperature of hydrogen was first reported by Benesch et al. in 1984 [6], and has been reported since by several independent groups around the world. Mills et al. reported extreme broadening in different plasmas, including RF discharges, microwave plasmas and glow discharges [7]. Our group at Eindhoven University of Technology measured extreme line broadening in RF discharges (Driessen [8]) and in DC glow discharges (De Maat [5]). Konjević, Kuraica et al. reported extreme broadening in many experiments (see [9] for a review).

There is a debate about the cause of the line broadening. Mills suggests a highly controversial model referred to as the *resonance transfer model*, based on the Blacklight process. Konjević and Kuraica suggest a model based on more standard physics, referred to as the *collision model*. Both groups claim their experimental results disprove the other's model. Both models give a qualitative description of the broadening, but fail to give a full quantitative description.

Extreme line broadening is discussed in detail in the Master's theses of Benjamin de Maat [5], Ruud Wijtvliet [10] and Niels Driessen [8].

1.1.3 EUV radiation

According to Mills et al. plasmas containing hydrogen produces EUV photons under certain conditions. Experimental results of EUV emission lines in a microwave plasma with helium and hydrogen are published in [11, 12, 13]. To the authors knowledge no independent confirmation of these results is published.

According to Mills the EUV radiation is produced in a series of emission lines with energies

\[ E = q \cdot 13.6 \text{ eV} \quad q = 1, 2, 3, \ldots \] (1.1)

The first lines of this series are shown in table 1.1. Not all lines in this series have been found experimentally. Lines are reported with $q = 1, 2, 3, 7, 9, 11$. See also figure 1.2.

When helium is added to the plasma, this leads to a second series. A dominant transition of helium is from He(1$s^2$) to He(1$s^12p^1$) with an energy of 21.22 eV (that corresponds to a very strong emission line at 58.4 nm). This transition of He supposedly absorbs part of the energy that otherwise would go to the EUV photon. This leads to lines with energies

\[ E = q \cdot 13.6 - 21.22 \text{ eV} \quad q = 2, 3, 4, \ldots \] (1.2)
Table 1.1: Series of emission lines in the EUV produced according to Mills [11]. From (1.1) and (1.2). Numbers in italic have been observed experimentally.

<table>
<thead>
<tr>
<th>q</th>
<th>$E$ (eV)</th>
<th>$\lambda$ (nm)</th>
<th>$E$ (eV)</th>
<th>$\lambda$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.598</td>
<td>91.176</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>27.197</td>
<td>45.588</td>
<td>5.979</td>
<td>207.373</td>
</tr>
<tr>
<td>3</td>
<td>40.795</td>
<td>30.392</td>
<td>19.577</td>
<td>63.331</td>
</tr>
<tr>
<td>4</td>
<td>54.394</td>
<td>22.794</td>
<td>33.176</td>
<td>37.372</td>
</tr>
<tr>
<td>5</td>
<td>67.992</td>
<td>18.235</td>
<td>46.774</td>
<td>26.507</td>
</tr>
<tr>
<td>6</td>
<td>81.590</td>
<td>15.196</td>
<td>60.372</td>
<td>20.537</td>
</tr>
<tr>
<td>7</td>
<td>95.189</td>
<td>13.025</td>
<td>73.971</td>
<td>16.761</td>
</tr>
<tr>
<td>8</td>
<td>108.787</td>
<td>11.397</td>
<td>87.569</td>
<td>14.158</td>
</tr>
<tr>
<td>9</td>
<td>122.386</td>
<td>10.131</td>
<td>101.168</td>
<td>12.255</td>
</tr>
<tr>
<td>10</td>
<td>135.984</td>
<td>9.118</td>
<td>114.766</td>
<td>10.803</td>
</tr>
<tr>
<td>11</td>
<td>149.582</td>
<td>8.289</td>
<td>128.364</td>
<td>9.659</td>
</tr>
</tbody>
</table>

Figure 1.2: EUV spectrum of a microwave plasma of a helium-hydrogen mixture (98/2%) (top curve) and control hydrogen (bottom curve). Source: Mills et al. [11].
1.2 Outline

Lines are reported from this second series with $q = 4, 6, 8$ (figure 1.2).

All three articles [11, 12, 13] are supported with the same few spectra, one of which is shown in figure 1.2. The spectra are made with a normal incidence EUV spectrometer (McPherson Model 302). Kunze [14] argues that this type of spectrometer is not suited for this spectral range, and that “the observed lines therefore must be artifacts.”

More recently, in 2008, Mills put a report on his website [15]. This report gives an overview of several spectroscopic observations. It has not been peer reviewed. The series of lines previously reported are missing, but instead two broad features are reported. The first is a continuum in a pulsed H$_2$ plasma which Mills associates with the $4 \cdot 13.6$ eV line at 22.8 nm, see figure 1.3(a). The second is a broad line at 63.3 nm in a He/H$_2$ microwave plasma which according to Mills corresponds with $3 \cdot 13.6 - 21.2$ eV, see figure 1.3(b).

The EUV photons are radiated in a process in which—according to Mills [16]—an electron is accelerated. Mills suggests that in the process one or several EUV photons are emitted with a total energy that is fixed according to the series in table 1.1. The resulting spectrum is a continuum that has an edge at the wavelength corresponding to that energy, and extends towards higher wavelengths. The maximum intensity of the continuum depends on the experimental plasma conditions. This process is similar to Bremsstrahlung.

1.2 Outline

In this thesis we will present a detailed discussion of the EUV spectroscopy experiments on plasmas containing hydrogen. We assembled two plasma sources, a microwave plasma and a pulsed plasma, and connected these to an EUV spectrometer. Chapter 2 contains a collection of theoretical subjects that are needed in the following chapters. The spectrometer will be discussed theoretically in chapter 3. The setup including the plasma sources will be discussed in chapter 4, followed by the experimental results (chapter 5) and discussion and conclusion (chapter 6). Deliberately we do not discuss Mills’s theory in the main text, since it is by no means accepted as standard physics, neither by us or the scientific world. For the curious reader we refer to the appendix A for an overview of the theoretical ideas of Mills. Appendix B is a general description of Fourier optics. Readers who are not familiar with this subject are advised to read this appendix before section 3.2.
Figure 1.3: EUV spectra with continuum radiation. Source: Mills et al. [15]
Chapter 2

Plasma theory

This chapter is a collection of theoretical subjects that are needed for this thesis. We will start with a general description of the hydrogen atom and the formation of emission lines. In section 2.2 we will discuss several broadening mechanisms of emission lines. In the last two sections we will describe the two types of plasma sources that we use in the experiments.

2.1 Energy states of hydrogen

Hydrogen consists of a heavy proton, with a much lighter electron orbiting it. The energy states of the electron in the hydrogen atom are a well known subject in physics. In first approximation they are given by the famous Bohr formula, (see [17])

$$E_n = -\frac{m}{2\hbar^2} \left( \frac{e^2}{4\pi \varepsilon_0} \right)^2 \frac{1}{n^2} = -13.6 \text{ eV} \frac{1}{n^2} \quad (2.1)$$

where \( n \) is the principal quantum number. The Bohr formula can be derived from the Schrödinger equation in a basic quantum mechanical system where a negatively charged electron orbits a positively charged, essentially motionless, proton.

<table>
<thead>
<tr>
<th>( n_2 )</th>
<th>Lyman series ( (n_1 = 1) )</th>
<th>Balmer series ( (n_1 = 2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>line</td>
<td>( \lambda ) (nm)</td>
<td>line</td>
</tr>
<tr>
<td>2</td>
<td>( \text{L}_\alpha )</td>
<td>121.567</td>
</tr>
<tr>
<td>3</td>
<td>( \text{L}_\beta )</td>
<td>102.572</td>
</tr>
<tr>
<td>4</td>
<td>( \text{L}_\gamma )</td>
<td>97.254</td>
</tr>
<tr>
<td>5</td>
<td>( \text{L}_\delta )</td>
<td>94.974</td>
</tr>
<tr>
<td>6</td>
<td>( \text{L}_\epsilon )</td>
<td>93.780</td>
</tr>
<tr>
<td>( \infty )</td>
<td>( \text{L}_\infty )</td>
<td>91.127</td>
</tr>
</tbody>
</table>

*Table 2.1: Emission lines of hydrogen in the EUV and the visible range. Source [18].*
The quantum number \( n \) has the integer values \( n = 1, 2, 3, \ldots \). With \( n = 1 \), the hydrogen atom is in its ground state with an energy of \(-13.6\) eV. Higher values of \( n \) are the excited states, with higher energies. The electron falls back spontaneously to lower excited states or the ground state. While it does, a photon is emitted, with a wavelength \( \lambda \) according to the Rydberg formula,

\[
\frac{1}{\lambda} = R_\infty Z^2 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)
\]

where \( n_1 \) and \( n_2 \) are the principal quantum numbers such that \( n_1 < n_2 \). \( R_\infty = 1.0974 \cdot 10^7\) m\(^{-1}\) is the Rydberg constant [19]. \( Z \) is the atomic number, which is 1 in case of hydrogen. This leads to series of emission lines that are characteristic for the hydrogen atom. When the electron falls back to the ground state (\( n_1 = 1 \)) we get a series of emission lines known as the Lyman lines. These emission lines have wavelengths which are in the EUV range. When \( n_1 = 2 \) this leads to the Balmer series which is mainly in the visible spectrum. See table 2.1.

The Rydberg formula also describes the emission spectrum of other hydrogen-line ions. These are ions with one electron: \( \text{He}^+ \), \( \text{Li}^{2+} \), \( \text{Be}^{3+} \) etc. with respectively \( Z = 2, 3, 4, \ldots \). This means for example that \( \text{He}^+ \) has a Lyman-like series of emission lines at a one fourth of the wavelength, and the Lyman \( \alpha \) line of \( \text{He}^+ \) for example is at 30.4 nm.

**Photon units**

Photons can be described in several ways. In this thesis the most common ways are to characterize them by their energy \( E \) or their wavelength \( \lambda \). They are related like,

\[
\lambda = \frac{hc}{E}
\]

where \( h = 4.135 \cdot 10^{-15} \) eVs is Planck’s constant, \( c = 2.998 \cdot 10^8 \) m/s is the speed of light in vacuum. Because the speed of light is not constant in different media, the wavelength varies with the refraction index. \( \lambda \) is usually in [nm] and \( E \) in [eV].

### 2.2 Line broadening

When measuring the spectrum of light that is emitted by a plasma, a line belonging to a certain transition is never perfectly at one wavelength, but rather spreads out over a range of wavelengths. There are several causes for this line broadening, which will be summarized briefly in this section. Line broadening is described in more detail in the thesis of Nienke de Vries [20].

\[\text{This means that the binding energy (the amount of energy that would have to impact to the electron in order to ionize the atom) of hydrogen in the ground state is 13.6 eV.}\]
2.2 Line broadening

The broadening of a line is often characterized by the Full Width at Half Maximum (FWHM), denoted as $\Delta \lambda$. The shape of the line profile depends on the mechanism that causes the broadening. The most common shapes are Gaussian and Lorentzian profiles. When different mechanisms cause broadening at the same time, the result is a convolution of the profiles. A convolution of a Gaussian and a Lorentzian is known as a Voigt profile.

2.2.1 Doppler Broadening

For us the most important type of broadening is Doppler broadening, or thermal broadening. When a particle that emits a photon travels with a certain velocity relative to the observer, the wavelength of the photon is Doppler shifted. The profile of the emission is determined by the velocity distribution in the plasma. Usually this is a Maxwell-Boltzmann distribution, which results in a Gaussian line profile. The FWHM of the Doppler broadening $\Delta \lambda_{\text{doppler}}$ is given (after De Vries [20]) by,

$$\Delta \lambda_{\text{doppler}} = \frac{\lambda_0 \sqrt{2 \ln 2}}{\sqrt{\frac{k_B T}{M c^2}}} \quad (2.4)$$

where $\lambda_0$ is the central wavelength of the unbroadered line, $T$ is the gas temperature, $M$ is the particle mass, $k_B = 8.617 \cdot 10^{-5}$ eV/K is the Boltzmann constant and $c = 2.998 \cdot 10^8$ m/s is the speed of light.

The Doppler broadening can be used to determine the gas temperature. This can best be done for light particles like hydrogen, and for large wavelengths (visible rather than EUV wavelengths).

2.2.2 Stark broadening

Stark broadening is an effect caused by the influence of nearby charged particles. It includes the effect of fast-moving electrons, which bombard the emitting particle, and the effect of slow-moving ions, which cause a shift of the energy levels. The exact treatment is complex, but in most cases Stark broadening has a Lorentzian shape. For hydrogen-like atoms an expression for the FWHM of the broadening $\Delta \lambda_{\text{stark}}$ in [pm] is (after De Vries [20]),

$$\Delta \lambda_{\text{stark}} = 1.23 \cdot 10^{-11} \alpha_{ij} n_e^{3/2} \quad (2.5)$$

where $\alpha_{ij}$ is the theoretical half width at half maximum that is dependent on the line, and $n_e$ in $[m^{-3}]$ the electron density.

Stark broadening is a type of pressure broadening, which is a collection of effects due to the presence of nearby particles. Other types of pressure broadening include resonance broadening and Van-der-Waals broadening. Usually these types of broadening are too small to be of any effect.
2.2.3 Natural line width

Broadening due to the natural line width is a direct effect of the Heisenberg uncertainty principle. It states that the energy and of an atomic state cannot be known with zero uncertainty if it has a finite lifetime. The FWHM of the natural broadening is usually in the order of 0.1 pm or less and is negligible compared to other broadening mechanisms.

2.2.4 Instrumental profile

Instrumental broadening is not caused by any physical effect in the plasma, but is due to the device used to record the spectrum. There are many causes for instrumental broadening, including the widths of the entrance and exit slit, the grating that is used, or focusing errors. A detailed discussion of our spectrometer can be found in chapter 3. Instrumental broadening usually has to be determined experimentally by measuring a line for which all other broadening mechanisms are small compared to the instrumental broadening.

2.3 Microwave plasma

A microwave plasma is a continuous plasma, in which the energy to sustain the plasma is provided by microwaves. The frequency of the microwaves usually is 2450 MHz. Nearly all applications for microwaves operate at this frequency. As a result sources are best available at this frequency and also other equipment is designed to work with 2450 MHz.

The energy of the microwave is transferred into the plasma by the charged particles, which are accelerated in the electric field of the microwave radiation. The heavy ions cannot follow the quickly alternating field, so most of the energy is transferred to the much lighter electrons. The fast electrons then transfer their energy by colliding with heavy particles, creating ions and excited particles. Microwave plasmas are energy efficient, since there is almost no direct heating of the background gas.

Several kinds of devices exist to transfer the microwave energy into the plasma, among which cavities, torches and launchers. For a description of different types see Wijtvliet [10], section 2.1. In our experiments, we use an Evenson cavity. More information on the Evenson cavity can be found in section 4.2 and is given by Fehsenfeld [21].

2.4 Pulsed plasma

Another method to create a plasma is to make a pulsed discharge between two electrodes. The electrodes are typically arranged cylinder-symmetrically. The electrodes are connected to a battery of capacitors, which acts as a power supply. The
2.4 Pulsed plasma

![Figure 2.1: Schematic picture of a basic Z-pincha discharge. The magnetic field $\vec{B}$ and the current $\vec{I}$ cause a Lorentz force acting on the plasma inwards.](image)

capacitors are in turn charged by an external high voltage power supply. The plasma is ignited in a way that depends on the specific type of plasma. After ignition the plasma is further ionized by Ohmic heating.

2.4.1 Pinch effect

During the discharge there is a current $\vec{I}$ flowing through the plasma in axial direction, which causes a magnetic field $\vec{B}$ in the azimuthal direction (see figure 2.1). The current is carried by the electron and ions in the plasma, which have a non-zero average velocity. The magnetic field causes a Lorentz force acting on these moving charges which is directed towards the axis of symmetry of the discharge. This causes the plasma to compress, an effect which is known as a Z-pincha.

The compression is balanced by the thermal pressure that causes the plasma to expand. This thermal pressure is caused by either Ohmic or compressional heating of the plasma. Also a decrease of the current ends the compression. This can happen by the pinch itself, which causes an increase of the plasma inductance and resistance, or as a result of the inherent oscillating nature of the current in an RLC circuit.

A basic Z-pincha design is shown in figure 2.1. The discharge happens between two electrodes that both have a hole in them. The discharge starts near the insulating wall, and moves to the symmetry axis due to the pinch effect. Two additional components are needed to operate the plasma. First, to stabilize the discharge, some form of active pre-ionization of the background gas is needed. And secondly, to build up the potential between the electrodes fast enough a spark-gap switch is needed.

Several types of pinch plasmas are described by Neff et al. [22] and in the thesis of Erik Kieft [23], pages 24-32. One of them is a hollow cathode discharge.
Hollow cathode triggered discharge

The design of a hollow cathode triggered discharge consists of two parallel plate electrodes at small distances, both with a hole in them. It differs from the normal Z-pinch design by a volume behind the cathode acting as a hollow cathode. This is shown in figure 2.2. The hollow cathode acts as a so-called pseudospark switch, and therefore the discharge can be operated without a separate spark-gap switch. Also there is no need for pre-ionizing the background gas.

Operating gas pressure and plate distance are such that the mean free path of the electrons for ionization is larger than the distance between the electrodes. This means that the no discharge takes place directly between the plates. The electric field—which is too high between the plates for effective ionization—penetrates the hole in the cathode, causing a weak field inside the hollow cathode. Free electrons are generated in the hollow cathode, which initiate a discharge between the plates. From there the evolution of the discharge is similar to that of other Z-pinch discharges.

The breakdown phase of the discharge is described by Kieft [23] and extensively by Boeuf et al. [24].
Chapter 3

Concave grating spectrometer

A spectrometer is a device that separates light into its wavelengths. In order to do this the light that enters the spectrometer through an entrance slit must be dispersed and focussed onto an exit slit or CCD. For extreme ultraviolet (EUV) wavelengths the transmittance or reflectivity is very low for all materials. Therefore the number of optical components must be kept to a minimum. Both the dispersion and the focussing is done by a grating.

For EUV spectroscopy we use in our experiments a spectrometer with a concave grating. In this chapter we will first discuss the dispersing and focussing properties of this type of spectrometers in a geometrical theory. Then we will discuss the grating in more detail with use of Fourier optics. This is a convenient method to show the effect of grating imperfections and other causes of spectral impurities.

3.1 Geometrical theory

Let us do a small thought experiment. Imagine two points anywhere in space and a randomly shaped surface, flat or otherwise. Let the two points emit a spherical wavefront with a certain wavelength. These wavefronts will both intersect the surface. At some points on the surface they will constructively interfere, while at other points they will destructively interfere. The surface can then be etched in such a way that the points with destructive interference will absorb light, and the points with constructive interference will reflect or transmit light. A spherical wave coming from one point that falls on the etched surface will be partially reflected or transmitted in such a way, that the resulting wave will constructively interfere in the other point. Effectively the surface focuses the light from one point into the other point. In an experimental setup the point sources are replaced by an entrance slit and an exit slit, and the edged surface is what is called a grating. We can conclude from this, that for any given entrance and exit slit, in principle it is always possible to
construct a grating that focuses a certain wavelength coming through the entrance slit onto the exit slit.\footnote{The slits need not even be points sources, but can be extended sources. In fact any source will do. If as ‘entrance slit’ a plain wavefront is taken, while the ‘exit slit’ is a 3-dimensional object, the resulting ‘grating’ is what is better known as a \textit{hologram}.}

Although theoretically any configuration of slits is possible, the manufacturing of a high quality grating poses some limits to the setup. With this in mind we will put two restrictions to our configuration. First, the grating must have a spherical surface. And secondly, the rulings on the grating must be equidistant. Such a configuration is shown in figure 3.1. Point $A(x_a, y_a, z_a)$ is the entrance slit and $B(x_b, y_b, z_b)$ is the exit slit. $P(x_p, y_p, z_p)$ lies on the spherical grating surface with radius $\rho$. $O$ is the center of the grating, and the origin of the coordinate system.

### 3.1.1 Light path function

The theory of concave gratings is already in 1945 extensively described by Beutler [25]. In the following we will present the basis, but we will skip the part where the algebra gets messy.

For the case of a spherical grating with equidistant rulings we will derive a geometrical theory. First we will write down some equations that follow directly from figure
3.1 Geometrical theory

Figure 3.2: Grating surface with rulings. The spherical surface has rulings with constant distance \(d\) along a chord. Also the blaze angle (see section 3.2.1) is constant with respect to that chord.

3.1 which we will need later on. The grating surface with radius \(\rho\) is given by,

\[
\rho^2 = (x_p - \rho)^2 + y_p^2 + z_p^2 \tag{3.1}
\]

From this quadratic equation \(x_p\) can be solved,

\[
x_p = \rho \pm \sqrt{\rho^2 - y_p^2 - z_p^2} \tag{3.2}
\]

Since the grating covers only a part of the sphere, we only need to consider half of the solution; the \(\pm\)-sign can be replaced by a \(\neg\)-sign. The optical path consists of two straight lines, \(AP\) and \(BP\), whose lengths are expressed by,

\[
AP^2 = (x_a - x_p)^2 + (y_a - y_p)^2 + (z_a - z_p)^2 \\
BP^2 = (x_b - x_p)^2 + (y_b - y_p)^2 + (z_b - z_p)^2 \tag{3.3}
\]

Furthermore the following holds,

\[
\begin{align*}
x_a &= r_a \cos \alpha \\
y_a &= r_a \sin \alpha \\
x_b &= r_b \cos \beta \\
y_b &= r_b \sin \beta
\end{align*} \tag{3.4}
\]

The grating is ruled with lines which run in the \(z\)-direction and with a constant distance \(d\) from each other. More precise, the rulings are equidistant as seen from far away (see figure 3.2), thus along the \(y\)-axis, and not along the grating surface. The condition for \(B\) to be a focus point, is that the light arriving in \(B\) must have a constant phase for all possible \(P\) along the ruled surface. The phase is given by the light path function \(F\),

\[
F = AP + BP + m\lambda \frac{y_p}{d} \tag{3.5}
\]

where \(\lambda\) is the wavelength, \(m = 0, \pm 1, \pm 2, \ldots\) is the order of the focus, and \(d\) the distance between the rulings. If \(B\) is to be the focus point, then \(F\) must be constant as \(P\) wanders along the grating, or,

\[
\begin{align*}
\frac{\partial F}{\partial y_p} &= 0 \tag{3.6a} \\
\frac{\partial F}{\partial z_p} &= 0 \tag{3.6b}
\end{align*}
\]
This condition is known as Fermat’s principle. It states that the path between two points by a ray of light is such as to make its optical path stationary with respect to variations of the path.\(^2\) If the light path function is satisfied, the optical path difference between two rays that are reflected by consecutive lines on the grating is integer times \(\lambda\). The light thus arrives in \(B\) with the same phase.

To calculate \(F\) we must evaluate \(AP\) and \(BP\) using equations (3.2), (3.3) and (3.4). This involves several series expansions and some elaborate algebra. Here we will give only the result, for the full treatment the reader is encouraged to read Beutler [25] or Namioka [26]. The terms of the expansions are expressed as

\[
AP = AP_1 + AP_2 + AP_3 + \cdots m\lambda \frac{y_p}{d} \tag{3.7}
\]

The expansion seems somewhat cumbersome, but the different terms have physical meaning. The first few terms are (after Beutler [25]),

\[
AP_1 = r_a - y_p \sin \alpha \tag{3.8a}
\]

\[
AP_2 = \frac{1}{2} y_p^2 \left( \frac{\cos^2 \alpha}{r_a} - \frac{\cos \alpha}{\rho} \right) \sum_{n=0}^{\infty} y_p^n \left( \frac{\sin \alpha}{r_a} \right)^n \tag{3.8b}
\]

\[
AP_3 = \frac{1}{2} z_p^2 \left( \frac{1}{r_a} - \frac{\cos \alpha}{\rho} \right) - \frac{z_p z_a}{r_a} + \frac{z_a^2}{2r_a} \tag{3.8c}
\]

\[
AP_4 = \frac{1}{2} z_p^2 y_p \left( \frac{\sin \alpha}{r_a} \right) + \frac{y_p \sin \alpha}{2r_a} \left( 2z_p z_a + z_a^2 \right) \tag{3.8d}
\]

\[
AP_5 = \left( \frac{y_p^2 + z_p^2}{8\rho^2} \right) \left( \frac{1}{r_a} - \frac{\cos \alpha}{\rho} \right) \tag{3.8e}
\]

\[
BP_1 = r_b - y_p \sin \beta \tag{3.9a}
\]

\[
BP_2 = \frac{1}{2} y_p^2 \left( \frac{\cos^2 \beta}{r_b} - \frac{\cos \beta}{\rho} \right) \sum_{n=0}^{\infty} y_p^n \left( \frac{\sin \beta}{r_b} \right)^n \tag{3.9b}
\]

\[
BP_3 = \frac{1}{2} z_p^2 \left( \frac{1}{r_b} - \frac{\cos \beta}{\rho} \right) - \frac{z_p z_b}{r_b} + \frac{z_b^2}{2r_b} \tag{3.9c}
\]

\[
BP_4 = \frac{1}{2} z_p^2 y_p \left( \frac{\sin \beta}{r_b} \right) + \frac{y_p \sin \beta}{2r_b} \left( 2z_p z_b + z_b^2 \right) \tag{3.9d}
\]

\[
BP_5 = \left( \frac{y_p^2 + z_p^2}{8\rho^2} \right) \left( \frac{1}{r_b} - \frac{\cos \beta}{\rho} \right) \tag{3.9e}
\]

\(^2\)Fermat’s principle is better known as the light following the minimum optical path. There are however situations where the light follows the maximum optical path, or one of many possible paths. The general principle therefore states that the optical path must be stable.
3.1 Geometrical theory

3.1.2 Grating equation

If only the first expansion terms are considered, the light path function $F$ is,

$$F = AP_1 + BP_1 + m\lambda \frac{y_p}{d} = r_a + r_b - y_p (\sin \alpha + \sin \beta) + m\lambda \frac{y_p}{d}$$  \hspace{1cm} (3.10)

Next we apply Fermat’s principle $\frac{\partial F}{\partial y_p} = 0$, equation (3.6a), and we get,

$$\sin \alpha + \sin \beta = \frac{m\lambda}{d}$$  \hspace{1cm} (3.11)

This is the well known grating equation. For a flat grating ($\rho, r_a, r_b \to \infty$) this equation is exact, since all higher order terms are 0. On the other hand, it holds for concave gratings too. It gives the condition for the focussing of wavelengths for different angles of incidence and diffraction.

3.1.3 Rowland circle

For a concave grating the higher order terms do not cancel out. They have to be taken into account when designing the geometry of a concave grating spectrometer, for they determine where the focus points will be. For this we apply Fermat’s principle to the second terms of $F$,

$$\frac{\partial (AP_2 + BP_2)}{\partial y_p} = 0$$  \hspace{1cm} (3.12)

$$\frac{1}{2} y_p \lim_{n \to \infty} (n+2) y_p^n \left( \left( \frac{\sin \alpha}{r_a} \right)^n \left( \frac{\cos^2 \alpha - \cos \alpha}{\rho} \right) + \left( \frac{\sin \beta}{r_b} \right)^n \left( \frac{\cos^2 \beta - \cos \beta}{\rho} \right) \right) = 0$$  \hspace{1cm} (3.13)

One simple solution for this equation is

$$r_a = \rho \cos \alpha \quad \text{and} \quad r_b = \rho \cos \beta$$  \hspace{1cm} (3.14)

This is the equation of a circle in polar coordinates. The circle is tangent to the grating surface and has a radius which is half the radius of the grating curvature ($\frac{1}{2}\rho$). What this means is that entrance slit $A$ and exits slit $B$ must lie on this circle. See figure 3.3. The circle is called the Rowland circle$^3$. It is named after H.A. Rowland, who described the theory of concave gratings for the first time in 1883 [27]. It is a key design feature for concave grating spectrometers. If the entrance slit is on the Rowland circle, the diffracted wavelengths will be brought to a focus also on the Rowland circle.

The most simple type of spectrometer that uses the Rowland circle is the Paschen-Runge mounting. It is this mounting that we use in our experiments. Typical to the Paschen-Runge mounting is that the grating and the entrance slit are fixed, positioned such that the entrance slit is on the Rowland circle. The spectrum is measured by either scanning the exit slit along the Rowland circle, or constraining a

$^3$In three dimensions the Rowland circle is in fact a cylinder, which extends in the z-direction.
Figure 3.3: The Rowland circle is a circle tangent to the grating with diameter $\rho$, which is the radius of the grating curvature. If the entrance slit $A$ lies on the circle, the focus points of the grating $B$ will also be on the circle.

CCD or—in the old days—a photographic plate to fit the Rowland circle. We use the Paschen-Runge mounting with the entrance slit positioned such that the incidence angle on the grating is grazing. This is needed to measure a spectrum with high resolution at low wavelengths (<100 nm).

There exist several more mountings based on the same principle, for example the Rowland mounting, designed by Rowland himself. In this mounting the grating and the exit slit (or photographic plate) are fixed on opposite sides of the Rowland circle. In the Eagle mounting the angles of incidence and diffraction are equal, or very nearly so. Other mountings are based on a different solution of equation (3.13). An example is the Wadsworth mounting, which uses a collimated incidence beam. More on different mountings can be found in [28], pages 228-232.

In the spectrometer that we will use, moving the exit slit will be done by controlling the distance between the grating and the exit slit $r_b$. It is therefore important to know the relation between $r_b$ and the wavelength $\lambda$ of the focus point. This can be calculated easily using the grating equation (3.11) and the relation,

$$\cos \beta = \frac{r_b}{\rho}$$  \hspace{1cm} (3.15)

This leads to,

$$\lambda(r_b) = \frac{d}{m} \left( \sin \alpha - \sin \left( \arccos \frac{r_b}{\rho} \right) \right)$$  \hspace{1cm} (3.16)

which can be also written as,

$$\lambda(r_b) = \frac{d}{m} \left( \sin \alpha - \sqrt{1 - \left( \frac{r_b}{\rho} \right)^2} \right)$$  \hspace{1cm} (3.17)
It may be of interest to know that the wavelength $\lambda$ is proportional to the distance $BC$ in figure 3.3.\(^4\)

### 3.1.4 Imaging errors

The higher order terms of the light path function $F$ are the cause of imaging errors.

**Astigmatism**

The terms $AP_3$ and $BP_3$ (equations (3.8d) and (3.9d)) are responsible for astigmatism. This is when a point source at point $A$ is not focussed as a point at $B$, but as a line. It can be shown that the length $L$ of a line that is the focus of a point source is (after Beutler [25]),

$$L = H \left( \sin^2 \beta + \sin^2 \alpha \frac{\cos \beta}{\cos \alpha} \right)$$

(3.18)

where $H$ is the height of the grating. The astigmatic error will increase with high angles $\alpha$ and $\beta$. For a grazing incidence spectrometer the error can become quite large, since $\sin \alpha \approx 1$. In the zero order $\alpha = \beta$ the astigmatism then becomes $L \approx 2H$.

This line is in the $z$-direction, perpendicular to the Rowland circle. It will therefore not cause any decrease of resolution. But it will spread out the light over a larger area, and thus decreases the intensity.

**Line curvature and coma**

The terms $AP_4$ and $BP_4$ (equations (3.8e) and (3.9e)) give rise to line curvature and coma. When a slit is used that is longer than a point source, the focus is a line. Due to an effect called coma this line is curved, rather than straight. Furthermore, every point on the slit produces a focal line as a result of astigmatism. Due to an effect known as curvature, this line is generally also not straight, but curved. The two curves are not necessarily of the same shape or even of the same sign. The results is that the two curves are convoluted (see figure 3.4). This does give rise to a loss

---

\(^4\)Some mountings, like the Rowland mounting, use this property. In the pre-computer age this would make the analysis more practical. Nowadays this advantage is of lesser importance, and the Rowland mounting is now indeed very rarely used.
of resolution. A quantitative description is cumbersome and difficult, and will be omitted here.\(^5\)

The terms \(A_P^4\) and \(B_P^4\) dependent on \(z_p\) and \(z_a\), and curvature and coma can be minimized by decreasing the height of the grating and the height of the entrance slit. Also decreasing the height of the exit slit can improve the loss of resolution to a certain extent, because only the center of the curved image is detected.

**Abberation**

The terms \(A_P^5\) and \(B_P^5\) (equations (3.8e) and (3.9e)) cause aberration, which is analogous to spherical aberration of lenses. \(A_P^5 + B_P^5\) must be smaller than \(\lambda/4\), otherwise an image cannot be formed. Since \(A_P^5\) and \(B_P^5\) depend on \(y_p^2 + z_p^2\), the size of the grating causes the aberration. This poses a limit to the size of the grating. To achieve maximum theoretical resolution on a grazing incidence spectrometer the width of the grating \(W\) must be (after Mack et al. [29]),

\[
W = 2.36 \left( \frac{4\lambda \rho^3 \cos \alpha \cos \beta}{\pi (1 - \cos \alpha \cos \beta) (\cos \alpha + \cos \beta)} \right)^{1/4}
\]

(3.19)

For \(\rho = 2217\) mm, \(\alpha = 82^\circ\) and \(\lambda = 100\) nm, the optimal grating width for the first order diffraction is \(W = 46\) mm. (The grating that we use in our spectrometer is circular with a diameter of 63 mm.)

### 3.2 Fourier optics of a diffraction grating

In the geometrical theory described above all the components were taken to be ideal. The slits were points with zero width, and the grating was perfectly spherical with equidistant rulings. The imaging errors derived are a direct result of the geometry of the spectrometer. In reality however, optical components are not perfect. This introduces a new type of errors in the spectrum due to diffraction on the grating. In this section we will discuss these effects.

A convenient way to discuss the diffraction of light by a grating is with Fourier optics. In Fourier optics a Fraunhofer diffraction pattern is described by a Fourier transform of the amplitude distribution function of a grating (or any aperture in general). Readers who are not familiar with this subject are advised to read appendix B.

The complex amplitude of the light coming from the grating (the grating distribution function) is \(u(x)\), where \(x\) is the position on the grating. The (complex) ampli-

\(^5\)Furthermore, according to Namioka [26] the quantitative treatment of coma and curvature by Beutler [25] is incorrect.
3.2 Fourier optics of a diffraction grating

The amplitude distribution of the diffraction pattern is \( U(\xi) \), with \( \xi \) the position on the diffraction pattern. \( U(\xi) \) and \( u(x) \) are related by,

\[
U(\xi) = C \int_{-\infty}^{\infty} u(x) e^{-i 2\pi \xi x} dx
\]

Aside from a constant phase factor \( C \) preceding the integral, this expression is the Fourier transform of the grating distribution function, evaluated at spatial frequency \( f = \xi/R\lambda \). In general the Fourier transform must be done in two dimensions \((x \text{ and } y)\), but for now the one-dimensional case is sufficient.

3.2.1 The concave diffraction grating

The diffraction pattern of the grating is described by the Fourier transform of the grating, when in the Fraunhofer regime. The grating itself is about 6 cm in diameter. With a wavelength of about 100 nm the distance to the grating needs to be larger than 36 km (see equation B.1 on page 81). This is clearly not the case, so for Fraunhofer diffraction to be valid the waves from the grating must be focused. As we have seen in section 3.1 the working of the concave grating can be split into different terms which are responsible for 1. diffraction according to the grating equation, 2. focusing onto the Rowland circle, and 3. imaging errors. This means that if we look at the diffraction pattern on the Rowland circle, and we ignore imaging errors, we can use Fraunhofer diffraction as if the grating were flat.

Flat grating

The most simple gratings consist of a collection of closely spaced grooves. The grooves reflect or transmit light, while the space between the grooves absorbs the light. The width of a groove is \( b \) and the distance between two grooves is \( d \). Ideally the grooves have infinitely small width \((b \to 0)\), and the amplitude distribution resembles a comb function (defined in equation (B.20), page 85).

\[
u(x) = \text{comb} \left( \frac{x}{d} \right) \quad \rightarrow \quad U(\xi) = C \cdot \text{comb} \left( \frac{d \xi}{R \lambda} \right)
\]

The Fourier transform is also a comb function. The diffraction pattern has different orders with \( m = 0, \pm 1, \pm 2, \pm 3, \ldots \), corresponding to the peaks of the comb function. The position \( \xi \) of a peak with order \( m \) corresponds to the wavelength as follows,

\[
\xi = R m \lambda / d
\]

This simple linear relation between \( \xi \) and \( \lambda \) is what makes gratings so useful.

At least two aspects are unrealistic about this ideal grating. First the grooves cannot be infinitely small, or only an infinitely small portion of the light is reflected. Secondly the grating cannot be infinity large, for obvious reasons.
Incorporating the finite groove width is done by convoluting the comb function with a rectangular function. According to equation (B.11) this means multiplying the fourier transforms by a sinc function (B.16). For groove width \( b \) this is,

\[
     u(x) = \text{comb}\left(\frac{x}{d}\right) \otimes \Pi\left(\frac{x}{b}\right) \rightarrow U(\xi) = C \cdot \text{comb}\left(\frac{d \xi}{R \lambda}\right) \cdot \text{sinc}\left(\frac{b \xi}{R \lambda}\right)
\]

The sinc function is broad with a width proportional to \( 1/b \). It acts as an envelope for the comb function. The intensity of the central order \( m = 0 \) is unaffected, but higher orders are decreased in intensity. Depending on the slit width, some orders may not be visible at all. But if the grooves become too wide, the sinc function becomes too narrow, and even the first order is diminished in intensity. Up to the point where \( b = d \) and the grating acts as a plane mirror. But on the other hand the grooves need to be as wide as possible, because all the light that falls between them is lost. This problem can be overcome by blazing, which we will come to in a moment.

The size of the grating can be taken into account by multiplying the amplitude function with a rectangular function of width \( W \). This envelope is expressed in the diffraction pattern as a convolution of the transforms.

\[
     u(x) = \text{comb}\left(\frac{x}{d}\right) \otimes \Pi\left(\frac{x}{b}\right) \otimes \Pi\left(\frac{x}{W}\right) \rightarrow U(\xi) = C \cdot \text{comb}\left(\frac{d \xi}{R \lambda}\right) \cdot \text{sinc}\left(\frac{b \xi}{R \lambda}\right) \otimes \text{sinc}\left(\frac{W \xi}{R \lambda}\right)
\]

This equation is shown graphically in figure 3.5. The diffraction pattern now no longer consists of sharp delta peaks, but of a series of sinc functions with a width proportional to \( 1/W \). This limits the resolving power of the grating, because different peaks of nearby wavelengths can overlap, making them indistinguishable. Moreover the peaks will have secondary maxima. One has to be careful that these secondary peaks accompanying a very bright peak are not mistaken for real peaks.

**Blazed grating**

One problem with the above grating, is that the zero order is always the strongest. And since this order contains no wavelength information, it is useless. There is however a way to shift the most intense order, so more light goes into a useful spectrum. This is done by, instead of a flat groove surface, putting the reflective surfaces under
an angle (like the grating in figure 3.2). The angle between the reflective surface and the mean grating surface is called the **blaze angle**, denoted as $\theta$.

Most high quality gratings are made the old-fashioned way, and that is by carving a pattern in a grating with a sharp diamond tip. This is called ruling, and the grating plus ruling tip are shown in figure 3.2.

Due to the relieved surface, the light that falls on different places of the grating has a slightly different optical path. What the blazing effectively does is introducing a linear phase change $\phi$ to the amplitude distribution. The groove width of a blazed grating is not only described by a rectangular function, but has an additional phase factor $e^{i\phi(x)}$.

Usually the blazing properties of a grating are given for the situation where light incidents perpendicular to the blazed surface, or $\alpha = \theta$. This is called the **Littrow condition**. In that case the extra optical path is $2x \sin \theta$. The phase change $\phi$ for the Littrow condition is,

$$\phi(x) = \frac{2\pi}{\lambda} 2x \sin \theta$$  \hspace{1cm} (3.25)

Multiplying the distribution function by a linear phase factor means convoluting the diffraction pattern by $\delta(\xi - 4\pi \sin \theta / \lambda)$. This convolution results in a shift of the envelope sinc function by $4\pi \sin \theta / \lambda$. The distribution function of one groove with width $b$ and its Fourier transform then become,

$$u_{\text{groove}}(x) = \Pi \left( \frac{x}{b} \right) e^{i \frac{4\pi \sin \theta}{\lambda} x} \quad \rightarrow \quad U_{\text{groove}}(\xi) = C \cdot \text{sinc} \left( \frac{b\xi}{\lambda} - \frac{2b \sin \theta}{\lambda} \right)$$  \hspace{1cm} (3.26)

With a blazed grating, there is no reason why the grooves should not be as wide as possible to get the most reflected light. This is when $b = d$, in other words there is no space between the grooves. To see which wavelengths are reflected the best by the grating, we have to substitute equation (3.22) into the envelope function. And since we are most interested in the first order, we take $m = 1$, resulting in,

$$U(\lambda) = C \cdot \text{sinc} \left( 1 - \frac{2d \sin \theta}{\lambda} \right)$$  \hspace{1cm} (3.27)

The square of this amplitude is the intensity, which is plotted in figure 3.6. This function is not constant, which means that a blazed grating is optimized for a particular wavelength. This wavelength with maximum intensity is called the **blaze wavelength**, which is at $\lambda = 2d \sin \theta$. This is only valid for the Littrow condition $(\alpha = \theta)$. Generally the blaze wavelength for an incident angle $\alpha$ is given by,

$$\lambda_{\text{blaze}} = d (\sin \alpha + \sin (2\theta - \alpha))$$  \hspace{1cm} (3.28)

The intensity decreases rapidly for wavelengths lower than the blaze wavelength, but for higher wavelengths the intensity falls more gradually.
3.2.2 Spectral impurities

In an ideal case one would expect light only to be diffracted into directions determined by the grating equation. In practice however there are several possible sources of stray light, which each give rise to a different form of unwanted scatter in the spectrum. These spectral impurities are shown graphically in figure 3.7. We will discussed them here briefly.

Diffraction effects

The first three impurities of figure 3.7 are a direct result of the finite grating size as described earlier, only here for the two-dimensional case. The diffraction pattern of a square grating (a) and a circular grating (b) are shown, as well as the effects on the spectrum. (c) shows the case where a grating is not uniformly illuminated, but with a Gaussian intensity distribution. The resulting diffraction pattern is the Fourier transform of a Gaussian, which is a Gaussian. The width of the diffraction pattern is inversely proportional to the width of the intensity distribution.

Ghosts

Spurious images known as ghosts are caused by periodic variations in the position or shape of the grooves on the grating surface. These errors are a result of the manufacturing process. Two types of ghosts can be distinguished: Long-term errors with a period in the order of the grating size. These errors cause images known as Rowland ghosts, and lie close to the main diffracted orders. Lyman ghosts on the other hand are caused by short-term errors with a period of a few grooves. They are found further away from the parent line.

The periodic errors in the grating behave as a grating in its own right, and the spectrum of this ‘error’ grating is then convoluted with the spectrum of the main grating. Ghosts are a genuine spectral image and have the same shape as the parent line, and the intensity is relative to that line.
3.2 Fourier optics of a diffraction grating

Perfect grating of finite width uniformly illuminated, square aperture.

Perfect grating, circular aperture, uniformly illuminated

Perfect grating, underfilled with Gaussian intensity distribution

Ghosts

Rowland

Lyman

Satellites due to imperfect wavefront

Grass

Diffuse scatter

Surface plasmon scattering

Figure 3.7: Forms of spectral impurities. Adapted from [28], page 142.
Satellites

Another form of grating defects are not periodic, but cover a substantial fraction of the grating. These are for example large scratches in the grating surface. These errors distort the Fourier diffraction pattern, which affects the central maxima, and distorts also the secondary maxima in both position and intensity. This gives rise to *satellites*, images that somewhat resemble Rowland ghosts, but differ in the fact that they are not symmetrically about the main order.

Grass

Short-term random errors in the grating surface give rise to scattered light further away from the main order. This can be for example a variation of the position of identical grooves, that is the errors occur in the direction perpendicular to the grooves. The light will be distributed in a line perpendicular to the grooves and will be seen as a faint background joining the diffracted orders. This is known as *grass*. Grass can be seen as the sum of the ghosts caused by many periodic Fourier components of the random distribution of errors.

Diffuse scattering

If the short-term random errors have no preferred direction, the light will just be scattered in any direction. The pattern of this diffuse scattering will be convoluted with the main spectrum. This type of scattering is caused by roughness of the grating surface, small scratches or dust.

Surface plasmon scattering

A final form of stray light, called *surface plasmon scattering* is due to a complex interaction between the electromagnetic field of the incident light, the conduction electrons of the metal and the roughness of the grating surface. It depends on the material of the grating surface and the polarization, and is beyond the capabilities of the transform approach. An extensive treatment can be found in Raether [30].
Chapter 4

Experimental setup

The setup that we use for our experiments consists mainly of three parts. The first part is the plasma source. We use two different sources: a microwave cavity and a pulsed plasma source. The source is connected to the second part of the setup, the EUV spectrometer. We use a grazing incidence concave grating spectrometer. Connected to the spectrometer is the third part, the detector. We can detect single photons using a Channel Electron Multiplier (CEM). All three parts are kept at low pressure by a vacuum system. This system will be discussed first. The three parts will then be discussed separately. Finally we discuss how we measure a spectrum.

4.1 Vacuum system

Wavelengths below 200 nm are absorbed by all gases. Thus to measure EUV radiation, it must travel through vacuum all the way from the plasma to the detector. The plasma, the spectrometer and the detector are connected through the entrance and exit slits of the spectrometer. The setup with the microwave source is drawn in figure 4.1. The slits have only a small surface, and although there is some additional leakage around the slits, the three parts of the setup are pumped separately. The three sections have pumping units that consist of a roughing pump and a turbo pump in series. This allows us to maintain a pressure difference between the compartments of 2-3 orders.

4.1.1 Flow controllers

Connected to the plasma compartment are two mass flow controllers of the type BRONCKHORST HITEC F-201C-FBC-33V. They control the amount of gas that flows into the system. One flow controller is connected to a bottle of hydrogen, while the other is connected to either argon or helium. The operation regime is between 2 and 100 sccm (standard cm$^3$/min) adjustable in steps of 0.1 sccm. The flow controllers are calibrated for oxygen with an input pressure of 2 bar. To get the correct flow rates
in sccm for other gases, the values can in good approximation be multiplied with a constant factor (see table 4.1).

<table>
<thead>
<tr>
<th>gas</th>
<th>factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrogen</td>
<td>1.028</td>
</tr>
<tr>
<td>argon</td>
<td>1.427</td>
</tr>
<tr>
<td>helium</td>
<td>1.433</td>
</tr>
<tr>
<td>hydrogen/helium (5%/95%)</td>
<td>1.400</td>
</tr>
</tbody>
</table>

4.1.2 Pressure sensors

All three compartments (plasma, spectrometer and detector) are fitted with full range pressure gauges of the type Pfeiffer Vacuum PKR 251. The gauge has two separate measurement systems: a Pirani and a cold cathode system, the signals of which are combined in such a way that one uniform measurement signal is output. This signal is logarithmic with pressure. This results in a sensor with a high range of $10^{-8}$-100 mbar, an accuracy of ±30% and a reproducibility of ±5%, according to the specifications for air or nitrogen. The measured pressure is dependent on the gas type, and can be off with a factor as high as 6 (for He below $10^{-5}$ mbar). Since we used this type of gauge only to get an indication of the order of the pressure, we did not correct for different gas types.

The accuracy of the full range sensors is sufficient for the spectrometer and the detector compartments, but the pressure of the plasma is needed with higher accuracy. Therefore an additional pressure meter was mounted near the plasma. This is a capacitive pressure sensor of the type Pfeiffer Vacuum CMR 363. This sensor
4.2 Microwave plasma source

We generate a microwave plasma inside a quartz tube that is part of the vacuum system. Around the tube a cavity is fitted to couple the microwaves into the plasma. In our experiments, we used an Evenson cavity (OPTOS INSTRUMENTS INC.).

The Evenson Cavity (shown in figure 4.2) consists of a hollow conductor that reflects the microwaves as to make a standing wave. The cavity needs to be tuned for two reasons. First the reflected power back to the generator must be minimized. This ensures that the standing wave has the maximum amplitude and the power can be most efficiently transferred to the plasma. Secondly the standing wave must have its maximum amplitude at the location of the quartz tube. If not the power dissipation in other parts of the cavity can cause overheating, or a plasma could be formed outside the tube. Two tuning adjustments are provided: a threaded tuning stub projecting into the cavity from the top, and a tuning handle that slides along the center conductor of the input connector. Also a tube is mounted on the cavity, to which a pressurized air connection can be fitted for cooling. For a detailed discussion of the Evenson cavity see Fehsenfeld [21].

The energy transfer to the plasma only works when there are free electrons present. To ignite the plasma these free electrons need to be created by a spark. A simple kitchen spark igniter proved to be sufficient provided the cavity is well tuned.

The power source is a microwave generator (MICROTRON 200 from ELECTRO MEDICAL SUPPLIES), connected to the input of the cavity by a coaxial cable with standard type-N connectors. The generator can provide up to 200 W microwave power, with a maximum of 50 W reflected power. Two indicators on the generator show the forward and reflected power. We used these values to determine the power input of the plasma, although the accuracy of these indicators is not known.
4.3 Pulsed plasma source

The second plasma source that we used is a pulsed discharge. The discharge happens between two electrodes, a cathode and an anode. The cathode is hollow, and we can assume that it is a hollow cathode triggered discharge. This is confirmed by the fact that the discharge can be spontaneously triggered, without the use of a spark gap switch or pre-ionization of the background gas. The discharge causes a quick voltage drop and therefore it lasts only for a short time (ca. 400 ns). See also section 2.4. The setup shown in figure 4.3 was designed and built by Blacklight Power Inc. We thank them for lending us this plasma source.

The anode and the cathode are two disks with 2-4 mm space between them. The metal must have a high resistance for discharges. We used two types of electrodes, made of molybdenum (Mo) and of tungsten-copper (WCu). Both the anode and the cathode have a hole in the middle (ø 3 mm), through which the discharge can be seen. The plasma source is connected to the entrance slit of the spectrometer at the red arrow pointing left in figure 4.3. It is important that the electrodes, the entrance slit and the grating are aligned in a straight line. To align the setup, a laser

Figure 4.3: Drawing of the pulsed plasma source. The yellow part indicates the high voltage part.
is used. A glass stub seals the vacuum behind the cathode. A small laser must be aimed through it, through the electrodes and the slit, onto the grating. This way one can make sure the setup is properly aligned.

To be sure that the gas composition between the electrodes is constant, the flow controllers are connected to a tube such that the gas input is directly between the electrodes (indicated by the blue arrow pointing down in figure 4.3). The gas flow is mainly through the anode, towards the spectrometer, since on this side the pumps are connected.

The electrodes are put in parallel with an array of high voltage capacitors (see right side of figure 4.4). The capacitors (20 of each 5.2 nF) have a total capacity of 104 nF. They are charged with a high voltage power supply (KILOVOLT CORP) that generates –15 kV. During the discharge the capacitors send a high current through the plasma. It is important that the connection between the electrodes and the capacitors has very low resistance and inductance. The plasma source is designed so that the capacitors are positioned close to the electrodes. The voltage of the cathode is measured with the use of a high voltage probe (NORTH STAR HV PVM-1 @ 1000:1). The probe reduces the voltage with a factor 1000, so it can be measured with an oscilloscope.

4.3.1 Electron beam

When the voltage over the electrodes is high enough, the discharge triggers spontaneously. But to have a better control over the rate at which the discharge happens, it can also be triggered. For this we use a beam of electrons aimed at the anode. When the anode is hit by electrons, and electrons enter the space between the electrodes, the discharge is triggered.

The e-beam is generated by an electron gun like the ones that are used in CRT television screens. The e-gun consists basically of a wire that emits electrons when heated. The heating is done by a battery, which has a circuit to adjust the voltage to a maximum of 24 V. The battery and the e-gun are electronically floating, and connected to a high voltage pulse generator (see the left side of figure 4.4). The HV
Experimental setup

4.3.2 Plasma power input

The voltage of the cathode and the voltage of the e-gun during a discharge are measured with the voltage probe and an oscilloscope (AGILENT 54624A). The result is shown in figure 4.5. It shows that the voltage on the cathode before the discharge is $-13 \text{kV}$. The voltage rises from $-13$ to $0 \text{kV}$ in $0.08 \mu\text{s}$ and oscillates for about $2 \mu\text{s}$. After that it builds up again for the next discharge. The oscillations are a common effect known as ringing. When the voltage rises above $-10 \text{kV}$ the oscilloscope generates a trigger signal that is used to start time resolved measurements (see section 4.7.3).

We know that the capacitance $C = 104 \text{nF}$, the voltage $V = -13 \text{kV}$ at the start of the discharge and the voltage rises to 0 in approximately $\Delta t = 80 \text{ns}$. We can estimate the current $I$ during the first part of the discharge,

$$I = \frac{CV}{\Delta t} = 17 \text{kA}$$  \hspace{1cm} (4.1)
It is difficult to know the amount of pinching, and therefore the size of the plasma.
We estimate that the plasma has approximately the size of the holes in the electrodes, which have a surface $A$ of $7 \text{ mm}^2$. The current density $J$ is approximately,

$$J = \frac{I}{A} = 2.4 \text{ GA m}^{-2}$$  \hspace{1cm} (4.2)

The energy $E$ that goes into one pulse is,

$$E = \frac{1}{2} CV^2 = 9 \text{ J}$$  \hspace{1cm} (4.3)

### 4.4 EUV spectrometer

The spectrometer we used is a MINUTEMAN LABORATORIES MODEL 322G, see figure 4.6. It was generously donated to us by the plasma physics group of the Ruhr-Universität Bochum, for which we are thankful. We named the spectrometer the ‘Kunze spectrometer’, after professor Hans-Joachim Kunze. The model is no longer in production, but similar to the present McPherson MODEL 247.

The spectrometer is a grazing incidence EUV spectrometer of the Paschen-Runge type. It has a Rowland circle with a diameter of $2.217 \text{ m}$. When the spectrometer is in operation, the grating and entrance slit are fixed, while the exit slit slides along the Rowland circle. The grating is mounted in a replaceable holder. Every grating has its own holder. This eases replacement of the grating. If an aligned grating is taken out and placed back afterwards, only very minor realignment is necessary.

The slits have variable widths, which can be continuously adjusted from $10 \mu\text{m}$ to $2 \text{ mm}$ with an accuracy of $5 \mu\text{m}$. This can be done while the slits are under vacuum. Also the height of the slits can be adjusted by masks in a range of $10 \text{ mm}$. For this the slit assembly must be opened, and cannot be under vacuum. The entrance slit
can be locked in discrete positions with incidence angle $\alpha$ adjustable from 82° to 88° with 0.5° increments. The position of the entrance slit on the Rowland circle is specified to be accurate to within 3 µm. The position of the exit slit can be controlled continuously by a high precision mechanism that is connected to a motor. There is also a knob to move the slit manually. However, this is not recommended, due to stress on delicate mechanical parts. The original motor was replaced by us with a stepper motor that can be controlled by a computer. This allows us to automate spectrum measurements. The motor is connected to a gear box. With the current stepper motor, there is no reason to change the gear ratio, which should be 5.

4.4.1 Alignment

When aligning the spectrometer, the goal is to position the slits exactly on the actual Rowland circle that is determined by the grating radius of curvature.\(^1\) Because the paths of the slits are fixed by the design of the spectrometer, the aligning procedure is the other way around: the grating is aligned to the Rowland circle of the apparatus.

The apparatus has micrometers on the slit holders and on the grating holder to accurately position the slits and the grating. First the slits must be positioned so that the device Rowland circle is corrected for small deviations of the grating curvature. Then the grating must be positioned so that the entrance slit is focused onto the exit slit.

For the course alignment of the grating a laser is directed perpendicular to the grating surface, through a hole in the vacuum chamber of the spectrometer. The fine alignment is done with an arbitrary light source in front of the entrance slit. The grating is aligned using the zero order. For the best result the alignment procedure has to be repeated for different angles of incidence. A ‘recipe’ with alignment instructions can be found in the instruction manual of the spectrometer. When done carefully, the entrance slit can be focussed onto the exit slit nearly perfectly. The system is then limited by the imaging errors described in section 3.1.4.

4.4.2 Mechanical error and range

The rotation of the motor (i.e. the amount of steps) is proportional to the distance between the grating and the exit slit $r_b$ (see figure 3.3 at page 24). As shown in equation (3.17) the wavelength $\lambda$ in [nm] can be calculated from $r_b$ by,

$$
\lambda = \frac{10^6}{f m} \left( \sin \alpha - \sqrt{1 - \frac{r_b^2}{\rho^2}} \right)
$$

where $r_b$ is the distance between the center of the grating and the exit slit in [mm], $f$ is the grooves/mm of the grating, $m$ is the order ($m = 1$ unless otherwise stated),

\(^1\)The radius of curvature of the grating is the diameter of the Rowland circle. See also chapter 3.
\[ \frac{\partial \lambda}{\partial r_b} = \frac{\Delta \lambda_{\text{mech}}}{\Delta r_b} = \frac{10^6}{f m \rho} \frac{r_b}{\sqrt{\rho^2 - r_b^2}} \]  

(4.5)

Here \( \Delta r_b \) is the error in the positioning of the exit slit\(^2\). \( \Delta \lambda_{\text{mech}} \) is the error in the wavelength due to errors in the positioning of the exit slit. \( \Delta \lambda_{\text{mech}} \) is plotted in figure 4.8 with \( \Delta r_b = 30 \mu m \), which is a realistic value for our spectrometer over the total range (see section 5.1.1). When measuring only a smaller wavelength range the error is much smaller (in the order of \( \Delta r_b = 1 \mu m \)). Therefore the mechanical error affects the position and repeatability of the central wavelengths of a peak, and much less the FWHM of the peak. The FWHM due to mechanical errors of the spectrometer is negligible compared to other effects, like slit widths (see below).

**Choice of grating**

Figures 4.7 and 4.8 show that the spectrometer has better resolution at low wavelengths. A grating with more grooves increases the resolution, but decreases the range of the spectrometer. A more grazing angle of incidence increases both range and resolution. However, with a more grazing angle, the projected surface of the grating decreases, and so will the intensity of the dispersed light. In the choice

\(^2\)This means that when the slit is moved to position \( r_b \), the actual position will be \( r_b \pm \Delta r_b \).
Experimental setup

4.4.3 Wavelength calibration

The motor of the spectrometer has a step counter with value $S$, with is related to $r_b$ by,

$$r_b = aS + b$$ (4.6)

$a$ and $b$ are constants that have to be found by calibration. $a$ is in mm/step. The value will not change unless the gear ratio or the hardware settings of the motor are changed, and normally there is no reason to do so. Therefore $a$ can be seen as a property of the spectrometer. The value of $b$ (in mm) changes more easily, when the slit is moved manually or when the step counter of the motor is reset to 0 due to a power loss. The calibration can be done with a light source that has known emission lines in the EUV range, for example a microwave plasma of helium or argon. $r_b$ can then be calculated with a known wavelength by using (4.4), solved for $r_b$, which is,

$$r_b = \rho \sqrt{1 - \left( f m \lambda \cdot 10^{-6} - \sin \alpha \right)^2}$$ (4.7)

4.4.4 Slit width

The width of the entrance slit and the exit slit can be adjusted continuously. Widening the slits causes more light to fall through the spectrometer, and thus increases
the signal. But wide slits also cause a decrease in resolution. The spectrum of a monochromatic light source is a peak with a finite width $\Delta \lambda$.

To calculate $\Delta \lambda$ we must look at the geometry of the spectrometer in figure 3.3 (page 24). The exit slit at point $B$ is parallel to the line $BC$. The length is given by,

$$BC = \sqrt{\rho^2 - r_b^2}$$  \hspace{2cm} (4.8)

Conveniently, this length is proportional to the wavelength $\lambda$,

$$\lambda = \frac{10^6}{fm} \left( \sin \alpha - \frac{BC}{\rho} \right)$$  \hspace{2cm} (4.9)

where $\lambda$ is in [nm] and $BC$ in [mm]. A slit with width $h$ catches all the wavelengths between $BC - \frac{1}{2}h$ and $BC + \frac{1}{2}h$. 3 The difference between those wavelengths is $\Delta \lambda$,

$$\Delta \lambda = \frac{h \cdot 10^3}{fm \rho}$$  \hspace{2cm} (4.10)

where we measure $h$ in [$\mu$m]. For a wide entrance slit the effect is the same. When the spectrometer is perfectly aligned, the focus of an entrance slit with width $h$ has also width $h$. When the (narrow) exit slit is scanned along this focus area, light from the wavelength is spread along the range between $BC - \frac{1}{2}h$ and $BC + \frac{1}{2}h$. The resulting $\Delta \lambda$ in the spectrum can be calculated in the same way.

When the entrance slit is narrow and the exit slit is wide, or visa versa, the spectrum of a monochromatic source will be a rectangular function with width $\Delta \lambda$. When the entrance slit and the exit slit are equally wide, the spectrum of a narrow line is the convolution of two rectangular functions, which is a triangular function with full width $2\Delta \lambda$. The FWHM however remains $\Delta \lambda$. In the general case of two different slits, the line broadening in [nm] of the spectrum due to the slits is given by,

$$\Delta \lambda_{\text{slits}} = \frac{h_{\text{max}} \cdot 10^3}{fm \rho}$$  \hspace{2cm} (4.11)

where $h_{\text{max}}$ is the largest of the two slit widths in [$\mu$m].

### 4.5 Visible spectroscopy

For the visible wavelength region we use two spectrometers: a DEMON for high resolution spectroscopy, and an Ocean Optics for quickly making a full range spectrum. The light is led to the spectrometers through an optical fiber, made of quartz. The coupling into the fiber is done by a lens, with a focal distance of 100 mm. With the microwave plasma the lens is positioned close to the cavity, aimed at the quartz tube. With the pulse source the lens is positioned in front of the glass view port. No special care is taken to focus the lens onto the plasma, because the intensity of the light is sufficiently high for both spectrometers. Darkening the lab during a measurement has almost no effect on the spectra, which means that the background noise from ambient light is negligible.

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3In fact this is valid for a slit that lies along the Rowland circle between $BC - \frac{1}{2}h$ and $BC + \frac{1}{2}h$. But the results for a small slit perpendicular to the grating are the same.
4.5.1 DEMON spectrometer

For high resolution spectroscopy of visible wavelengths we use a Double Echelle Monochromator (or DEMON). Figure 4.9 shows the inside of the spectrometer. The most important part of the DEMON is the echelle grating. An echelle grating is characterized by a relatively low groove density and a high blaze angle. It is used in the Littrow mounting\textsuperscript{4}. Therefore the diffraction pattern of the grating has its maximum intensity at a very high order (up to $m = 50$). At these order the dispersion is very high, and hence the spectrometer has a high resolution. One problem of looking at very high diffraction orders, is that the different orders overlap each other. This is solved by using a second monochromator to preselect a small wavelength region. The DEMON has a prism monochromator for this purpose.

Light enters the DEMON through a fiber, and falls on the entrance slit of the prism monochromator. By rotating the prism, the appropriate wavelength region falls through the exit slit of the prism monochromator, which is the entrance slit of the echelle spectrometer. The echelle grating disperses the light again and the high resolution spectrum is focussed on a CCD.

We use an ANDOR DV 434 CCD, with an array of $1024 \times 1024$ pixels with square pixels of 13.5 $\mu$m. The CCD is cooled to $-58^\circ$C, which leads to a negligible dark current. The horizontal pixels are used for measuring the spectrum, while the vertical pixels allow for measuring several channels simultaneously.

The DEMON has a total range of 200-900 nm. The wavelength range that is preselected by the prism spectrometer, and thus the range of one measurement, is 1 to 5 nm, depending on the wavelength. The resolution between two pixels of the CCD is respectively 1 to 5 pm. Measurements of the experimental profile are done by de Maat \cite{5}. The FWHM is specified to be 9.9 pm at 656 nm and 6.1 pm at 486 nm.

\textsuperscript{4}This means that the incidence angle equals the blaze angle.
4.6 Channel Electron Multiplier

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**Figure 4.10:** Working principle of a Channel Electron Multiplier

**Figure 4.11:** Drawing of a Channel Electron Multiplier

### 4.5.2 Ocean Optics spectrometer

We use the OCEAN OPTICS HR2000+ spectrometer for quickly measuring a full visible spectrum. The spectrometer is of the type Czerny-Turner (see Pedrotti [32], page 362). It has a range of 400-850 nm, with a resolution of 0.3 nm FWHM. The detector is a CCD with an array of 2048 pixels. A full spectrum can be measured at once with an integration time ranging from 1 ms to 20 s.

### 4.6 Channel Electron Multiplier

A Channel Electron Multiplier or CEM is a type of detector that can be used for the detection of ions, electrons or high energy photons like EUV or X-ray. The CEM that we use is the DETECTOR INC. MODEL 206-10C-SL. It consists of a hollow channel made of silicate glass that is processed to have secondary emissive and resistive properties. The channel is curved to prevent positive ions from traveling back to the input end of the channel. A cone is fitted at the front to catch particles. Two electrical connections are mounted to the channel, through which a large voltage...
Experimental setup

(2.4 kV) is applied to it. When a photon hits the side of the channel, it releases an electron. This electron is drawn towards the end of the channel by the voltage, and when it hits the side, secondary electrons are released (see figure 4.10). A cascade of electrons travels down the multiplier channel, causing a small current between the two electrodes that can be detected. The number of electrons that reach the end of the channel is called the gain, which for our detector is \(5.6 \times 10^7\).

Sometimes a cascade of electrons happens that is not triggered by an incoming photon or ion. This is known as dark count. The CEM has a specified dark count of less than 0.05 counts/s. This is negligible in all our experiments. The CEM needs a pressure of \(10^{-4}\) mbar or less to operate.

Measurements with the CEM can be performed in two ways. When few photons hit the detector, all the current pulses can be counted individually. This mode allows for the detection of single photons. When too many photons hit the detector, the pulses overlap and single photon counting is not possible anymore. Instead the current through the detector must be integrated. The integrated current is proportional to the number of the photons hitting the detector.

In our measurements we used only photon counting. Figure 4.12 shows how the CEM is connected. The front electrode of the CEM is grounded, while the back electrode is connected to a +2.4 kV power source. The signal at this point is low and noisy, which is why a discriminator is used. The input of the discriminator is shielded from the high voltage by a capacitor. When the discriminator detects a rising flank on its input that exceeds a preset adjustable threshold (the dotted line in figure 4.12), it outputs a clean TTL pulse. This TTL pulses can be counted by a counter unit that is connected to a pc. As discriminator we used the SIGNAL RECOVERY MODEL 1182. The output pulse has a preset adjustable width. When the pulse width is set to a minimum, the total dead time is 20 ns.

It is vital that the connections between the CEM and the discriminator are well shielded and the cables are as short as possible. The signal at this point is very weak (mV range), and any interference will be amplified by the discriminator and cause false counts.
4.6.1 Aluminum filter

A CEM is sensitive for photons with wavelengths below 200 nm. This makes it insensitive to noise from visible wavelengths. But \( \text{H}_2 \) has a lot of emission bands with wavelengths around 90-120 nm. These wavelengths can cause noise in the spectra when they hit the CEM as stray light. We can improve the signal to noise ratio of the spectra by installing a filter that blocks these wavelengths.

We use a filter of the type LUXEL 1500 Å AlTFT-111. The filter consists of a 150 nm thick aluminum film supported by a fine nickel mesh. It is mounted directly in front of the CEM. The transmission properties are shown in figure 4.13.

4.7 Counting system

The CEM measures EUV photons, which are translated into TTL pulses by the discriminator. In this section will be explained how we count these pulses and accumulate the actual data.

4.7.1 Dead time behavior

Each counter has a dead time \( \tau \) that limits the maximum count rate. This is the processing time that the counter needs after it has detected an incoming pulse.

Counters can be divided in two types of dead time behavior. In all cases a pulse that arrives during the dead time will not be counted. The first type of counter just ignores the pulse, and starts counting again after the dead time. This type is called

![Figure 4.13: Transmission plot of the Luxel 1500 Å Aluminum filter. Source: Luxel.](image)
Experimental setup

Figure 4.14: Illustration of the dead time behavior for two types of pulse counters. Of the total of 6 pulses the paralyzable counter counts 3 pulses, while the nonparalyzable counts 4.

A second type of counter has a dead time after each pulse, whether the pulse is counted or not. This type is called paralyzable. An example of the behavior of both types is shown in figure 4.14. For a complete treatment see Knoll [33].

At high count rates a correction of the measured data is needed. To calculate this correction we assume the distribution of the photons in time to be random\(^5\). For nonparalyzable counters the correction is given (after Knoll [33]) by

\[ I_m = \frac{I_t}{1 + I_t \tau} \]  

where \(I_m\) is the measured intensity (or count rate) and \(I_t\) is the true intensity. This equation is plotted in figure 4.15. Indeed for low intensities \(I_t \ll 1/\tau\) the measured value is accurate \(I_t \approx I_m\). At very high count rates \(I_t \to \infty\) the measured value approaches the maximum \(I_m \to 1/\tau\). Counters are often characterized by their maximum count rate \(I_{\text{max}}\), defined as,

\[ I_{\text{max}} = \frac{1}{\tau} \]  

Already at much lower count rates the measured counts differ from the true counts. For the error to be less than 10%, the count rate must be \(I_m < 0.1 \cdot I_{\text{max}}\).

Equation (4.12) can easily be solved for \(I_t\), so a correction is possible. Only the uncertainty will increase for high count rates.

For paralyzable counters the relation between the measured counts and the true counts is given (after Knoll [33]) by

\[ I_m = I_t e^{-I_t \tau} \]  

This equation is also plotted in figure 4.15. At low count rates the paralyzable case is approximately equal to the nonparalyzable case. The difference is the behavior at high count rates. The nonparalyzable counter has a maximum of \(I_m\) at \(I_t = 1/\tau\). At \(\tau\)

\(^5\)Poissonian to be precise.
4.7 Counting system

Figure 4.15: Measured and true count rates for two types of pulse counters. The count rates are normalized to the maximum count rate $I_{\text{max}}$.

even higher $I_t$, the measured rate $I_m$ decreases again, going to 0 ultimately. In this range the counter is said to be paralyzable. A consequence is that for each $I_m$ there are two possible $I_t$. Equation (4.14) can only be solved iteratively for $I_t$. Automated correction is therefore difficult.

The counters that we use are all of the nonparalyzable type. However, the discriminator is a paralyzable system. The discriminator generates TTL pulses, that can overlap if pulses follow each other too quickly. In that case the result is one broad TTL pulse. The counter that is connected to the discriminator sees only one rising flank, so only one pulse is counted.

4.7.2 Spectrum measurement

To measure the intensity of EUV light, the exit slit of the spectrometer must be moved to the appropriate wavelength and then the pulses from the CEM must be counted. To measure a spectrum this has to repeated many times for different wavelengths. To automate this process, we control both the motor that moves the slit and the counter by computer. The motor (a TRINAMIC PANDrive PD-109-57 stepper motor) can be controlled over an RS-232 connection. As a counter we used a TUEDACS Timer/Counter Unit. This counter has a maximum count rate $I_{\text{max}} = 10 \text{ MHz}$. It is connected to the computer by USB using a TUEDACS USB2.0 SERIAL HIGHWAY CONVERTER. The counter can be told to start counting pulses for a preset amount of time, after which it returns the number of counts. Both the motor and the counter are controlled by software that was specially written by us to be used with this spectrometer. This software uses equations (4.4) and (4.6) to calculate at which wavelength the exit slit is positioned. The output of the program is a text file with the number of counts and their corresponding wavelengths. The internal value $S$ of the stepper motor is also saved, so the spectrum can be manually recalibrated afterwards if necessary.
At low count rates \((I_t < 10 \, \text{MHz})\) the measurement system is limited by the TUe-DACS counter, and will behave as a nonparalyzable system with \(\tau = 100 \, \text{ns}\). At high count rates \((I_t > 50 \, \text{MHz})\) the discriminator will ‘paralyze’, and even though the dead time of the discriminator is shorter than of the TUeDACS counter, it will become the limiting factor. Then the counting system will behave as a paralyzable system with \(\tau = 20 \, \text{ns}\).

### 4.7.3 Multichannel Scaler

A second type of pulse counter that we use is a multichannel scaler (MCS). A MCS counts pulses as a function of time. When the MCS is started, it begins counting pulses in the first channel. After a preset dwell time it advances to the next channel, and so on. It thus builds up a histogram of counts as function of time.

We use the Ortec MCS-PCI, which is a PCI-card. The dwell time of a channel can be set to a minimum of 100 ns, and the maximum number of channels is 65,536. The start can be triggered externally, and the MCS can also be configured to trigger multiple times. This way the counts from several passes can be accumulated. The MCS has a maximum count rate \(I_{\text{max}} = 150 \, \text{MHz}\). But the internal clock of the MCS is 50 MHz based, and the counting can only start on a clock tick. This means that there is a 20 ns jitter between the trigger input and the actual start of the counting. The MCS comes with its own software, and at the moment it is not possible to control the stepper motor with this software.

The MCS has a smaller dead time than the discriminator, so for all count rates the system will be limited by the discriminator. The system will behave as a paralyzable system with \(\tau = 20 \, \text{ns}\). The different channels have no influence on the counting behavior. It is ensured that no counts are lost or counted double when the MCS switches between channels.

**Triggering the Multichannel Scalor**

With a channel width of 100 ns it is important that the MCS is triggered accurately every time at precisely the same moment of the discharge. We can not use the pulsed signal of the pulse generator of the e-beam, because there is a jitter of about 100 ns between the start of the e-beam pulse and the discharge. Therefore we use the voltage of the cathode to trigger the discharge. The output of the voltage probe is measured with an oscilloscope, which is used to detect the start of the discharge by triggering on the rising flank of the voltage. The trigger output of the scope is a positive TTL pulse, but unfortunately the MCS triggers on a falling slope\(^6\). Converting the trigger pulse into a negative pulse is done with a delay generator (Stanford Research Systems Inc. Model DG535)\(^7\). The output of the delay generator is  

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\(^6\)This appears to be a device bug. The manual tells that the MCS triggers on a rising slope, but it does not.

\(^7\)Using a delay generator to invert a pulse might seem overkill, but it was the quickest solution at the time.
used as a trigger for the MCS. This results in a total jitter between the discharge and the start of the MCS of less than 40 ns.

Although the jitter is within acceptable limits, the trigger signal has an inherent delay, which meant the MCS misses approximately the first 200 ns of the discharge. This is solved by delaying the pulse signal by 500 ns (and no jitter) with a long (50 m) cable between the discriminator and the MCS. The electronic setup of the MCS is drawn in figure 4.16.
Chapter 5

Experimental results

In this chapter the results of the spectroscopic measurements will be shown. We will start by discussing the results of the microwave plasma. This is a convenient plasma source to test the EUV spectrometer. For this we use gases with a known spectrum. Next we will present the results of a microwave plasma with He and H\textsubscript{2}. After that the results of the pulsed plasma source will be shown. We present spectra of H\textsubscript{2} and He, and also time resolved measurements.

5.1 Microwave plasma

The microwave plasma is generated inside a quartz tube with an Evenson cavity. The tube is connected directly to the entrance slit of the EUV spectrometer as shown in figure 4.1. The pressure inside the quartz tube is adjusted to 0.5 mbar in all the microwave experiments that are shown in this section. The microwave input power is set to 100 W, the reflected power varied between 5 and 50 W. The cavity is adjusted to have a minimum reflected power.

Spectra of the microwave plasma are made with the TUeDACS counter. The discharge is continuous, so no triggering is needed to start counting. The EUV intensity is relatively low; the count rate usually is below 10 kHz. In rare cases, at the top of strong emission lines, the intensity can be as high as several MHz. But by decreasing the slit width it is always possible to decrease the intensity to below 1 MHz, 0.1 times the maximum count rate. This means we do not have to worry about non-linear effects because of overlapping counts. Using the TUeDACS counter is convenient, because spectrum measurements can be automated. This makes a microwave plasma excellent for testing and calibrating the spectrometer.

5.1.1 EUV spectrometer calibration

All spectra from the EUV spectrometer in this thesis are made with a grating with $f = 600$ grooves/mm and a blaze angle of $2^\circ{}4'$, and with an angle of incidence $\alpha = 82^\circ$. 
The alignment is done as described in section 4.4.1. The aluminum filter is used, unless otherwise stated. For the calibration we use helium, because it has two series of emission lines between 23 and 30 nm and between 50 and 59 nm. A spectrum of He is shown in figure 5.1. The horizontal axis has already been calibrated to the wavelength, but the raw data is \( S \), the number of steps of the stepper motor. The linear relation between \( S \) and \( r_b \), the distance between the grating and the exit slit, has to be found by calibration according to equation (4.6).

In practice it is difficult to accurately measure \( r_b \) directly. Therefore we calculate \( r_b \) for various wavelengths using equation (4.7) for which we can determine \( S \). In the spectrum we identify several emission lines of He, for which \( r_b \) is calculated using known wavelengths from the NIST database [18]. Some of the peaks are identified as second or third order lines. A linear fit is made with the raw values for the position of the peaks \( S \) and the corresponding calculated values for \( r_b \). For \( r_b \) in [mm] the fit results in

\[
r_b = S(-4.7639 \pm 0.0002) \cdot 10^{-5} + 474.534 \pm 0.008
\]

(5.1)

The residue of this fit is shown in figure 5.2 on the vertical axis, plotted against the wavelength of the emission lines on the horizontal axis. The residue can be interpreted as the error in the position \( \Delta r_b \), caused by mechanical limitations of the spectrometer. It can be seen that \( \Delta r_b \) is less than 30 µm over a large wavelength range.

For higher wavelengths we operate the microwave plasma with a mixture of Ar/H\(_2\) (97/3%). The spectrum in figure 5.3 shows the Lyman series of H and several Ar and Ar\(^+\) lines. A linear fit (graph not shown) of the peaks of this spectrum yields,

\[
r_b = S(-4.765 \pm 0.001) \cdot 10^{-5} + 474.64 \pm 0.07
\]

(5.2)

The differences with the fit of the He spectrum are within the margin of error. The Ar/H\(_2\) spectrum is less accurate than the He spectrum for two reasons. First be-
5.1 Microwave plasma

Figure 5.2: Residue of a fit of peak positions from a He microwave plasma, plotted against wavelengths of emission line wavelengths taken from the NIST database [18] (multiplied by the diffraction order). The values can be interpreted as positioning errors of the exit slit.

cause the spectrometer has a better resolution at lower wavelengths, secondly—and most importantly—because larger slits were used in the Ar/H\textsubscript{2} measurements (50 µm against 10 µm for the He spectrum).

Instrumental profile

The instrumental profile of the spectrometer depends on several factor. There are the imaging errors (section 3.1.4), spectral impurities (section 3.2.2) and broadening due to slit width (section 4.4.4). Figure 5.4 shows high resolution spectra of a He line, taken with different slit widths. At larger slit widths the shape of the peak is triangular, which is as expected. At smaller slit widths the peak becomes narrower, and the intensity relative to the background increases.

Figure 5.4 also shows that the central wavelength of the peaks shifts. This is due to the mechanics of the spectrometer. The accuracy of the calibration decreases after several back and forth movement of the exit slit. It is found that the wavelength calibration is accurate to within 10 pm, even after many movements of the exit slit.

The theoretical value of line broadening by slits of 10 µm is 7.5 pm, according to equation (4.11). We measured a FWHM of 8 pm. An example of a He line at 53.703 nm is shown in figure 5.5. The shape of the peak is not triangular, therefore we fitted the peak with a Voigt curve. The shape of the peak is for the most part Gaussian (6.6 pm), and has a small Lorentzian part (1.6 pm). If the Gaussian part is caused by Doppler broadening, according to equation (2.4) the corresponding temperature of He (with mass 4.003 u) would be 1.6 \cdot 10^{5} K or 14 eV. This would be extremely high, and therefore the broadening is likely not to be caused by Doppler broadening, but
Experimental results

**Figure 5.3:** Microwave plasma with Ar/H$_2$ (97/3%). The peaks marked with * are Ar lines. The unmarked peaks are mostly molecular H$_2$ lines. The spectrum is taken without the aluminum filter.

**Figure 5.4:** He line at 52.2 nm measured with different slit widths. The intensities are normalized to the background level.
5.1 Microwave plasma

Figure 5.5: High resolution spectrum of He line in a microwave plasma. The peak is fitted with a Voigt curve, which has a Gauss width of 6.6 pm and a Lorentz width of 1.6 pm. Right shows a detail of left.

rather by instrumental broadening. Gaussian instrumental broadening can come from imaging errors and diffuse scattering by the grating.

It can also be seen that the peak is slightly asymmetrical, which could be caused by imaging errors like line curvature and coma. There is also a small peak visible at the higher wavelength side, with its center at 29 pm from the center of the He line. The small peak could not be identified as a spectral line. It is possible that this is a satellite peak, caused by grating imperfections. This would mean that this peak would also appear next to other peaks, with the same intensity ratio to the parent peak (which is $7 \times 10^{-3}$). We have not found this satellite peak near other peaks, although we have not extensively checked this. Most spectra were not taken with such high resolution.

5.1.2 Unidentified features in He/H$_2$ mixtures

We measured spectra of microwave plasmas of He and various mixtures of He and H$_2$. A detail of the He spectrum from figure 5.1 is shown in figure 5.6(a). There are several lines visible from impurities, mainly O$^+$. Several features in the spectrum could not be identified, including two broadened features around 57 nm and 66 nm.

H has no known emission lines below the Lyman series at 91.1 nm. Also molecular H$_2$ has no known lines below 78 nm (see Abgrall et al. [34]). These wavelengths are blocked by the aluminum filter. Therefore the spectra of He and a mixture of He and H$_2$ are expected to look identical. Indeed all the features in the He spectrum can also be found in the spectrum of a mixture of He and H$_2$ (see figure 5.6(b)), including the He and He$^+$ lines, lines from the impurity O$^+$ and other unidentified features. There is one difference however: a broad feature between 62.7 and 63.4 nm only appears in the He/H$_2$ microwave plasma.
Figure 5.6: Detail of spectra of microwave plasmas with He and a mixture of He and H₂. The peaks indicated with * are lines from O⁺ impurities.

Figure 5.7: He/H₂ (98/2%) microwave plasma with and without aluminum filter.
5.1 Microwave plasma

Figure 5.8: Microwave plasma of different mixtures of He and H$_2$. A feature around 63 nm appears only at low fractions of H$_2$. The peak at 64.1 nm is a second order He line.

Figure 5.9: Microwave plasma Ar/H$_2$ (97/3%). Spectrum taken without aluminum filter. No feature is visible.

Figure 5.7 shows this feature in more detail. The intensity of the peak does not change relative to the background when the aluminum filter is removed. This indicates that the peak is indeed caused by light of 63 nm. Unlike the other peak in the spectrum, which is a 2$^{nd}$ order peak of the 32.0 nm He line. The intensity of this peak increases relatively to the background when the filter is used. This is because the filter has a higher transmission at 32 nm than at 64 nm.

The peak around 63 nm is not visible in pure He, and neither in pure H$_2$. It is only visible in mixtures of He with a small fraction (<25%) of H$_2$. This is shown in figure 5.8. A mixture of Ar and H$_2$ also shows no feature, see figure 5.9.
Figure 5.10: Full range spectrum of a He/H\textsubscript{2} microwave plasma, measured with the DEMON spectrometer.

Figure 5.11: Spectrum of H\textsubscript{\textbeta} line in a He/H\textsubscript{2} microwave plasma measured with the Demon spectrometer (blue dots). The red curve is a Gaussian fit with central wavelength 486.1342 nm and FWHM 14.54 ± 0.07 pm.
5.2 Pulsed plasma source

Visible range spectra

In the visible range we measured a spectrum of the He/H\textsubscript{2} microwave plasma with the DEMON spectrometer. The results are shown in figure 5.10. This spectrum shows several lines from He and from H\textsubscript{2}. The unmarked lines are mostly lines from impurities, which is mainly oxygen.

The Balmer \( \beta \) line (486.133 nm in air [18]) is shown at high resolution in figure 5.11. The line is fitted with a Gaussian curve. The fit is not perfect, especially at the maximum and at the bottom the measured intensity does not follow the fit. A fit with a Lorentz curve was also tried, but the result was worse. A Voigt curve gave a zero Lorentz width, which is essentially the same results as a Gaussian fit. Also fitting with several Gaussians did not improve the fit. From the fit parameters the FWHM was determined to be 14.5 pm. Fully attributed to Doppler broadening this yields a temperature (equation (2.4)) of \( 2.4 \cdot 10^3 \) K or 0.21 eV. Taken into account that most likely not all broadening can be fully attributed to Doppler broadening, this is a normal value for a microwave plasma. No extreme line broadening is visible.

5.2 Pulsed plasma source

We connected the pulsed plasma source to the EUV spectrometer as described in section 4.3. The setup is aligned with a small HeNe laser to ensure that the holes in the electrodes, the entrance slit and the grating are in a straight line. The HV power source of the discharge is set to –15 kV. The e-beam, used for triggering, is adjusted to give a pulse of –2.9 kV at a rate of 5 Hz with a pulse width ranging from 0.5 to 2 ms. Two types of electrodes are used: molybdenum and tungsten-copper.

We measured spectra from the pulsed plasma source the same as we did with the microwave plasma; the pulses from the CEM are transformed by the discriminator, and counted by the TUeDACS counter. There are however several complications. First the discharge is not constant; the intensity varies from pulse to pulse. Secondly, the counting is not triggered by the pulse source. Therefore the amount of pulses in one measurement has a statistical variation of one pulse. Both problems can be minimized by integrating over many pulses.

A third problem cannot be overcome easily. Although in total less counts are produced than with the microwave plasma, the pulsed plasma produces very short, bright pulses. During those pulses the photon rate well exceeds 50 MHz, which is the maximum pulse rate of the discriminator. This causes the discriminator to paralyze the counting, and an increase of photon intensity will cause a decrease in the number of counts. This means that the spectra must be interpreted with caution. Quantitatively, because peak heights are not linear with the line intensity, and also qualitatively, because more counts does not necessarily mean higher intensity.

Besides the TUeDACS counter we use a Multi Channel Scaler (MCS) to measure the counts time resolved. In addition the MCS has a faster counter (150 MHz), which
Experimental results

improves the accuracy of the counting at medium count rates (approximately between 5 and 50 MHz). The MCS is set up to count for 10 µs and divide the counts into 1000 channels of 100 ns. The counts from a number of discharges (usually 2000) are accumulated in order to get enough signal. The beginning of each pass is triggered by the cathode voltage. See also section 4.7.3.

We also did visible spectroscopy. First we will discuss the results of H$_2$, followed by He. The slits of the EUV spectrometer are set 10 µm.

5.2.1 Pulsed H$_2$ plasma

H$_2$ is used in the pulse source with a pressure ranging from 0.8 to 1.2 mbar.

Figure 5.12a shows the spectrum of a pulsed plasma with pure H$_2$ with Mo electrodes, and figure 5.12b shows a spectrum made with W-Cu electrodes. In the spectra are many small peaks visible. These peaks are shown in more detail in figure 5.13, where two measurements were done under similar conditions. It shows that most of the peaks are reproducible. From this we can conclude that the peaks are not noise, but a feature of the plasma. Some peaks can be identified as lines of oxygen, mostly O$^{3+}$. Oxygen is also in pulsed plasmas a common impurity. Molybdenum and copper both have many emission lines in this wavelength range. But the ions must be highly ionized (Mo$^{5+}$ or Cu$^{4+}$ and above), and it is unsure if these ions exist in the plasma.

We smoothed the spectrum with a Savitzky-Golay filter. This filter fits a polynomial function of a certain degree through a window of points around a central point. The smoothed value of the central point is then based on this fit. Advantages of the filter are that it tends to preserve features such as local maxima and minima. We used the filter of order 3 and a window of 101 data points. The results are the red curves in figure 5.12.

The spectrum 5.12a shows a continuum with its left flank at 23 nm and extending to around 37 nm. In the spectrum 5.12b there are several features visible. There is a continuum visible with its left flank at 24 nm extending to 29 nm. The maximum of this continuum is about 2 nm further than the continuum in the previous spectrum, and the measured intensity is lower. Another continuum is visible at 32 nm extending to 37 nm. Note that the aluminum filter has a decreased transmission below 17 nm (see figure 4.13), so features in this region will likely not be visible.

The continuum radiation is visible when there is H$_2$ present in the plasma, even when it is only a very small fraction. If an experiment with pure He is undertaken after an experiment with H$_2$, it is needed to pump for about a day to remove impurities. Only then the continuum would disappear.
5.2 Pulsed plasma source

Figure 5.12: Pulsed plasma with H$_2$. The red curves show the results of a Savitzky-Golay filter (of order 3 and a 101 point window) applied to the spectrum.
Experimental results

Figure 5.13: Two spectra of a pulsed H$_2$ plasma made under similar conditions.

Time resolved measurements

We did time resolved measurements on the H$_2$ plasma under the same conditions as the spectrum showed in figure 5.12a. In this wavelength region there are no known lines of H or H$_2$, but some lines from impurities are visible. One of them is a line from O$^{3+}$ at 23.9 nm. The results of the MCS while the spectrometer was positioned at the top of this peak is shown in figure 5.14(a). 5.14(b) and 5.14(c) show measurements of the MCS at 21 and 25 nm respectively. It is checked by a quick scan with the TUeDACS counter that at these wavelengths there are no peaks. The exit slit is positioned at a local minimum of the spectrum. 21 nm is taken outside from what appears to be a continuum, while 25 nm is approximately at the maximum of the continuum.

There are several observations to be made. First the difference between an emission line and no emission line. The O$^{3+}$ line shows the characteristics of extreme paralysis of the counting system during the discharge: first a count rate of exactly 1 count/discharge followed by several channels with almost no counts. The actual photon intensity will likely be much higher. The measurements also show an afterglow which lasts until about 4 µs. The afterglow has two maxima, at 0.9 µs and 2.0 µs. Although the maximum at 0.9 µs might not be a real maximum, but a result of the counter that recovers from the paralyzed mode during the discharge. The two measurements with no emission line on the other hand show no afterglow. The counts are all produced during the discharge.

There is a difference in intensity of the discharge for measurements taken on the continuum and not on the continuum. Note the scale differences in figures 5.14(b) and 5.14(c). It thus seems that the radiation that causes the continuum is predominantly produced during the discharge, and not during the afterglow.

To check this several more measurements were done with the MCS on wavelengths with no emission lines. In the data from the MCS the first 700 ns were added up and plotted in figure 5.15. This figure only shows the counts that are produced during
5.2 Pulsed plasma source

Figure 5.14: Time resolved counting from pulsed H2 plasma. Data accumulated from 2000 discharges.
Experimental results

Figure 5.15: Intensity of discharge without the afterglow of a pulsed H\textsubscript{2} plasma. Each point is the sum of the first 700 ns (7 channels) of measurements with the MCS taken at different wavelengths. The points are taken at wavelengths with no emission lines.

Figure 5.16: Pulsed H\textsubscript{2} plasma measured with Ocean optics spectrometer. Peaks indicated with * are identified as Mo lines.

The discharge, without the afterglow. The result shows a continuum which is much clearer than the spectra made with the TUEDACS counter.

Visible spectrum

The H\textsubscript{2} pulsed plasma has also been studied by visible spectroscopy. A full spectrum is shown in figure 5.16. The Balmer series is visible. Also several other lines are visible, mainly from O and from Mo.
5.2 Pulsed plasma source

5.2.2 Pulsed He plasma

A pulsed plasma is made with He at a pressure ranging from 1.6 to 2.2 mbar. The spectrum made with the TUeDACS counter is shown in figure 5.17. It shows emission lines of He\(^+\), as well as second order lines of He\(^+\), and several lines from O\(^+\) impurities. Remarkably the He lines (which are very intense in the microwave plasma) are almost absent. The He\(^+\) series has reversed intensity; the line at 25.6 nm is stronger than 30.4 nm. This is most likely an effect caused by paralysis of the counter, which means that a higher intensity causes a decrease in count rate. This is confirmed by the relatively high intensity of the second order lines. This indicates that the measured intensity is not linear with the actual intensity. Why the He lines are so weak is explained by time resolved measurements.

Time resolved measurements

We measured with the MCS on several emission lines of He\(^+\). To do this first we made a quick high resolution scan of the emission line with the TUeDACS counter, after which the exit slit was positioned on the center of the peak. The results are shown in figure 5.18.

The graphs show the evolution of the discharge. The first 0.2 \(\mu\)s (2 channels) show few counts. This means that the counts are delayed such that the trigger pulse is 200 ns ahead of the discharge. The next 0.4 \(\mu\)s (4 channels) show a high count rate, with a maximum between 1.5 and 2 counts/discharge for all wavelengths. This is most likely the actual discharge, and the actual intensity is much higher than the maximum count rate. This causes the counting system to paralyze. An extreme
Figure 5.18: Time resolved counting of He⁺ lines in a pulsed He plasma. Data accumulated from 2000 discharges.
5.2 Pulsed plasma source

Figure 5.19: Time resolved counting of the He line at 58.4 nm in a pulsed He plasma. Data accumulated from 10000 discharges. Data from the first 300 ns of the discharge is missing.

example is visible in the figure 5.18(a). The MCS counts almost exactly 1 count/discharge in the beginning of the pulse, followed by several channels with almost no counts. What happens is that the discriminator produces one pulse per discharge that is as wide as the discharge due to the very high photon count. We checked with an oscilloscope that this is indeed the case.

After the discharge the signal decreases, and increases again. In the case of He\textsuperscript{+} lines, the afterglow of the discharge dies out after approximately 27 µs. In the afterglow radiation there is a structure with three maxima around 2.3, 4.3 and 7.8 µs. Most of the counts are measured during the afterglow.

The time evolution of the 58.4 nm line of He is also measured, see figure 5.19. Because of incorrect triggering the first 300 ns of the discharge are missing.\footnote{This is not the case in the He spectrum of figure 5.17, since there is no triggering with the TUeDACS counter. False triggering therefore cannot be the cause of the weak He lines.} It shows that there is very little afterglow. Because most counts that make the spectrum in figure 5.17 are produced in the afterglow, the He lines look very weak compared to the He\textsuperscript{+} lines.

Visible spectrum

The visible spectrum of a pulsed He plasma is shown in figure 5.20. The spectrum shows lines of He and He\textsuperscript{+}. Note that the He lines are not weak in this spectrum. The ocean optics spectrometer has a CCD, which does not paralyze at high count rates. The intensities are therefore more reliable than in the EUV spectra. Also quite strong Balmer lines from H are visible, which is an impurity in this measurement.

The Balmer α of H is measured at high resolution with the DEMON spectrometer. Although H is an impurity it is a strong line, that can be used to measure the Doppler broadening. The measurement with Gaussian fit is shown in figure 5.21. The fit has a width of 34 pm, which corresponds (according to equation 2.4) to a temperature of \(1.3 \times 10^4\) K or 1.14 eV. There is no extreme line broadening.
Figure 5.20: Spectrum of a pulsed He plasma made with the Ocean Optics spectrometer. * indicates He lines and + indicates He$^+$ lines. The unmarked lines are impurities, mainly Mo.

Figure 5.21: Pulsed He with H$_2$ impurities. Balmer $\alpha$ line measured with DEMON spectrometer (dots) and with Gaussian fit (red curve). The fit has a FWHM of 34 pm. The feature at 656.0 nm is a He$^+$ line.
Chapter 6

Discussion and Conclusion

6.1 Setup

We can conclude that the spectrometer is working properly. The accuracy of the wavelength calibration over the whole range of 2-113 nm is 10 pm. The resolution is limited mostly by the slit widths, which can be adjusted to a minimum of 10 µm. At the minimum slit width the peak shape is predominantly Gaussian, which indicates that the limit posed by the slits coincides with the limits of the grating. The instrumental profile has a FWHM of 8 pm, which is in agreement with theoretical predictions. The sensitivity of the spectrometer in combination with the Channel Electron Multiplier is high enough to see most known emission lines. For example in a microwave plasma of hydrogen we can detect the Lyman series up to \( L_\eta \).

The vacuum system works to our satisfaction. We can maintain a plasma with a pressure around 1 mbar and at the same time keep the pressure at the detector below \( 10^{-4} \) mbar, which is needed to operate the CEM. We have a good control over different gas mixtures, although there are always impurities present, mainly oxygen and hydrogen, most likely from \( \text{H}_2\text{O} \) from the wall of the vacuum vessel.

The system for photon counting works properly for the microwave plasma, but for the pulsed plasma source the maximum count rate is insufficient to accurately measure the intensity during the discharge. With the Multi Channel Scaler we can measure the intensity time resolved. In the first 400 ns of the discharge the intensity is still too high to give reliable results, but in the afterglow the intensity is below the maximum count rate.

6.2 63 nm peak of the He/H\(_2\) microwave plasma

In a microwave plasma of He we found lines from He, He\(^+\), O\(^+\) and a few unidentified features. A mixture of H\(_2\) and He shows the same spectrum, with one difference: a broad feature between 62.7 and 63.4 nm. This feature is interesting for two
reasons. First, it only appears in microwave plasmas with He and a small fraction of H\textsubscript{2} (<25%). At higher fractions the feature disappears. This makes it less likely that the feature is caused by an impurity.

Secondly, the cause of the feature is unknown, although it has been reported previously by Mills et al. under the same experimental conditions. Mills attributes the peak to a reaction with hydrogen which produces a photon, with an energy of \(3 \cdot 13.6 - 21.2\) eV. This would make a photon of 63.3 nm, which corresponds approximately (but not exactly) to the right flank of the peak. It is unknown why the peak is broadened, and why it is broadened mainly to lower wavelengths. To the knowledge of the author there are no other accounts in literature of a feature around 63 nm under comparable conditions.

He is known to have several continua (see Hill [35]). One of them is in the ultraviolet range between 60 and 110 nm, and is known as the Hopfield continuum. It has two maxima in the intensity at 79.3 nm and 68.5 nm and several local maxima (Huffman et al. [36]). The continuum is attributed by Tanaka [37] to the transitions from bound excited states of the He\textsubscript{2} molecule to its unstable ground state. The peak that we measure cannot likely be attributed to this continuum for two reasons. First the wavelength does not correspond to one of the maxima of the continuum, and the shape is different. Secondly the continuum does not explain why the peak would only appear in a mixture of He and H\textsubscript{2}.

The spectrum of He\textsuperscript{2+} also has continuum radiation, but this continuum is above 150 nm (see Hill [38]). If the 63 nm peak could be attributed to HeH (helium hydride) this would explain the He/H\textsubscript{2} mixture that is needed in the plasma. But HeH has no emission lines in the EUV range (see Ketterle [39]). Also HeH\textsuperscript{+} has no transitions with enough energy to emit light in the EUV range (Engel et al. [40]).

### 6.3 Afterglow of the pulsed He plasma

With the MCS we measured the emission of radiation time resolved. In a pulsed He plasma we measured that the afterglow last up to 30 µs, while the discharge is only 0.4 µs long. The afterglow is visible at emission lines of He\textsuperscript{+}, but absent at lines of He. The afterglow of He\textsuperscript{+} has a structure with several maxima.

Del Val et al. [41] used a pulsed plasma source similar to ours. They measured the electron density and the temperature time and space resolved. The time resolved temperature, electron density and the current through the plasma show a structure of about 250 µs long which is similar in shape to the structure we see in our measurements of the photon intensity. In our setup we did not measure the current directly, but the voltage of the cathode decreases to 0 after 2 µs. We can assume that there runs no current through the plasma after that. So even if a change in the photon intensity is caused by a change in temperature and electron density, this cannot be explained for our setup by a change in plasma current.
The fact that there is a difference in the afterglow of He lines and He$^+$ lines would suggest some kind of process that produces excited He$^+$. We did not look in detail at possible processes.

## 6.4 Continuum in the pulsed H$_2$ plasma

We measured a spectrum of a pulsed plasma with H$_2$. This spectrum shows a continuum between 23 and 37 nm with its maximum at 25 nm. Time resolved measurements with the MCS show that this continuum radiation is produced mainly during the discharge itself. It is, however, dangerous to draw conclusions from the intensity measurements during the discharge, because the photon count exceeds the maximum counting rate of the counting system. We measured a change in the spectrum when we changed the electrode material. A spectrum made with a WCu electrode shows a continuum which is much less clean. It is difficult to draw conclusions from this, because a change in plasma parameters could also be explained by a small change in the electrode distance.

Mills reports this continuum on his website [15]. He attributes the line to a reaction where a photon is released with an energy of $4 \cdot 13.6$ eV, or a wavelength of 22.8 nm. This corresponds to the left flank of the continuum. Mills proposes a process [16] similar to Brehmsstrahlung, which qualitatively explains the broadening of the line towards higher wavelengths. Apart from Mills there are to the author's knowledge no reports in literature of lines or continuum radiation of H or H$_2$ in this wavelength region.

## 6.5 Conclusion

The goal of the project was to verify the experimental results of Mills et al. in EUV spectroscopy. The most remarkable of these results are a series of lines in a He/H$_2$ microwave plasma, published in 2003 [11]. We were unable to reproduce these results, even though our microwave setup was very similar, and our spectrometer was even better suited for these EUV wavelengths. A more recent report (2008) from Mills [15] also omits these lines in the results. Two previously unknown features remain: a line at 63.3 nm in a He/H$_2$ microwave plasma, and a continuum between 23 and 30 nm in a pulsed H$_2$ plasma. Both these experimental results we were able to reproduce under the same conditions.

The explanation that Mills has for these results requires the acceptance of a controversial new type of reaction with hydrogen (see appendix A). Other arguments that are based on more standard physics cannot explain the results. Our measurements however, are in a wavelength region (<100 nm) which is relatively unexplored. It is not unthinkable that one of the species that is present in our plasma, as a result of some plasma reaction or as a contaminant, has an unknown line or continuum at one of the wavelengths that we have measured. Furthermore Mills only gives a
qualitative description. Some properties of the lines are not explained by Mills either, like the way the line at 63.3 nm is broadened. The fact that not all the lines are broadened in the same way would suggest that the underlying process is different. Also why some lines predicted by Mills are observed and others are not, is not explained.

6.6 Recommendations

For further research into this subject we can do the following recommendations.

**Improve the CEM measurements with current integration.** During the first 400 ns of the pulsed discharge, the results of the CEM are unreliable when used with photon counting, because the count rate exceeds the maximum count rate. The CEM acts as a current source, and integration of this current allows for much higher count rates to be measured. If the measurements of the continuum in the pulsed H₂ plasma could be verified using current integration, this would greatly increase the reliability of the results.

**Repeat the experiments with a self-built pulse source.** The pulse source that was used for the experiments is designed and built by Blacklight Power Inc. To claim complete independence from Mills et al. its is better to verify the results with a source that is built from scratch.

**Investigate molecular processes in the pulsed He plasma.** The measurements of the afterglow of He⁺ and He in a pulsed plasma suggest some sort of process in which excited He⁺ is formed. A possible process is suggested by Van Der Mullen [42]. The process involves the production of He²⁺,

\[
\text{He}^2+ + \text{He} \rightarrow \text{He}^2_2^+ \tag{6.1}
\]

The He²⁺ acts as a reservoir. With dissociative recombination excited He⁺ is produced,

\[
\text{He}^2_2^+ + e^- \rightarrow \text{He}^{++} + \text{He} \tag{6.2}
\]

It is not known if this process happens in the pulsed plasma, nor what the cross sections are. Further research in this and other processes is needed to draw any conclusions.
Appendix A

Theory of Mills

In the last few years Dr. Randell Mills and his company Blacklight Power Inc. has published several articles with experimental results. The explanation that Mills has for these results is based on a new type of reaction of hydrogen with a so-called catalyst. In this reaction, according to Mills, a new form of hydrogen is formed, that has an energy level below the ground state. A hydrogen atom in a state below the ground state is called a hydrino. According to standard quantum physics hydrinos cannot exist.

Hydrinos are a result of a completely new atomic theory that Mills has made, which he calls the Grand Unified Theory of Classical Physics (GUToCP). The theory is inconsistent with standard quantum physics, and for this reason Mills is widely criticized for his ideas. In this appendix we will give a small introduction of the theory, and present an overview of the criticism that faces it. It must be noted clearly that the theory described in this appendix represents the ideas of Randell Mills. The scientific world does not accept these ideas as valid physical theories. The fact that we describe Mills’s ideas must not be interpreted as an acknowledgement of them.

A.1 Publications about GUToCP

Mills has published his theory a number of times (see [43, 44] and more on the website http://www.blacklightpower.com), but ultimately all publications refer to his book [45]. This very extensive book consists of three volumes and covers more than 1700 pages. It has not been peer reviewed.

Only few sources are known that independently comment on Mills’s theoretical findings. The first is Rathke [46], who investigates the theoretical basis of hydrino states. His conclusion is that GUToCP “is inconsistent and has several serious deficiencies”.  

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1 First Mills named his theory Classical Quantum Mechanics (CQM) but because of some confusion with normal quantum mechanics he later adopted the name GUToCP.
Mills reacts to this [47], causing Rathke to publish an erratum (but not change his conclusion).

A second source is Naudts [48], who investigates the possibilities of hydrino states as a solution of the Klein-Gordon equation\(^2\) in quantum mechanics. This solution was already known in the early days of quantum physics, but rejected as being unphysical. As a reaction to this Dombey [49] and de Castro [50] again rejected the hydrino state by confirming the old point of view.

In addition Shechtman published a short communication [51], but he merely gives a summary of Mills's ideas and only proposes a change to one small detail of the hydrino theory.

### A.2 Hydrinos

The energy states of hydrogen according to quantum physics are given by the Bohr formula, equation (2.1). Mills claims his theory predicts the same energy states of the hydrogen atom, and additionally predicts fractional quantum states, with \(n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, \frac{1}{137}\).\(^3\) Mills calls these states hydrino states, with the energies of the first few states given in table A.1. According to quantum mechanics fractional quantum states are impossible. The question whether hydrinos exist is therefore highly controversial.

#### A.2.1 Blacklight process

Even though there exist states of lower energy, the ground state of hydrogen is stable according to Mills. This means the electron cannot fall back to a hydrino state by spontaneous emission of a photon. The hydrino states itself are also stable (i.e. non-radiative). Mills however says that it is possible to have a transition from the ground state to a hydrino state by nonradiative energy transfer. Hydrogen can transfer integer times its potential energy, or \(m \cdot 27.2 \text{ eV}\) where \(m = 1, 2, 3, \ldots\) during a reaction.

\(^2\)The Klein-Gordon equation is a relativistic variant of the Schrödinger equation in relativistic quantum mechanics.

\(^3\)The series is terminated at \(n = \frac{1}{137}\) because at lower fractions the energy would exceed the rest mass of the electron, making the total energy of the electron negative.
A chemical or physical process with a net enthalpy of $m \cdot 27.2 \text{ eV}$ can absorb this energy and act as a catalyst. An example is $\text{He}^+$, with a second ionization energy of $54.4 \text{ eV} = 2 \cdot 27.2 \text{ eV}$. The helium absorbs the energy from the hydrogen, leaving the hydrogen in an metastable state below the ground state. This is shown in figure A.1 and in the formula,

$$\text{H}(n=1) + \text{He}^+ \rightarrow \text{H}^* (n = \frac{1}{3}) + \text{He}^{2+} + e^- \quad \text{(A.1)}$$

The metastable state then decays to the nearest stable state, which is in this case is $n = \frac{1}{3}$.

$$\text{H}^* (n = \frac{1}{3}) \rightarrow \text{H}(n = \frac{1}{3}) + 54.4 \text{ eV} \quad \text{(A.2)}$$

The remaining energy is either emitted as a photon, or transferred to a second hydrogen atom to form fast hydrogen. The process of bringing the hydrogen in a hydrono state is called the Blacklight process.

There are many possible catalysts, including $\text{Ar}^+$, $\text{Sr}^+$, $\text{Li}$, $\text{K}$, $\text{Cs}$ and $\text{NaH}$. Two hydrogen atoms together can act as a catalyst in a three-body collision. Also the hydrono itself can absorb $m \cdot 27.2 \text{ eV}$ and can act as a catalyst. An extensive list of reactions with hydrono catalysts is given by Mills et al. in [13].

### A.3 The electron according to Mills

The GUToCP—the theory that predicts hydronos—rejects quantum mechanics. It states that atomic physics can be described by classical laws, like the laws of Newton, Maxwell and Einstein’s relativity. A traditional problem with these classical physics at atomic scales is that electrons inside an hydrogen atom are not stable,
but lose energy by radiation. The idea of Mills is that the electron is not a point source, but a two-dimensional charge distribution.

The basis of the theory is the bound electron. In the first chapter of his book [45] Mills describes the single-electron atom. The electron takes the form of a spherical shell with the nucleus in the center. Mills calls this the *orbitsphere*. The charge distribution of the orbitsphere $\rho$ is a superposition of spherical harmonics $Y_l^m(\theta, \phi)$. Mills gives the following expressions for $\rho$ (after [45]),

for $l = 0$

$$\rho(r, \theta, \phi, t) = \frac{e}{4\pi r^2} \delta(r - r_n) Y_0^0(\theta, \phi),$$

(A.3)

for $l \neq 0$

$$\rho(r, \theta, \phi, t) = \frac{e}{4\pi r^2} \delta(r - r_n) \left( Y_0^0(\theta, \phi) + \Re \left[ Y_l^m(\theta, \phi)e^{i\omega t} \right] \right),$$

(A.4)

where $e$ is the total charge of the electron and $\Re(\cdot)$ gives the real part. The orbitsphere has a total mass $m_e$. The electron spin is the result of a complicated pattern of current in the surface of the orbitsphere.

In a hydrogen atom in ground state the radius of the orbitsphere is the Bohr radius $a_0$. According to Mills excited states—characterized by their quantum number $n$—are orbitspheres of radius $n a_0$. Besides the well known states $n = 1, 2, 3, \ldots$, Mills argues that also states exist with $n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$. These are the hydrino states, which have a radius smaller than the Bohr radius.

### A.3.1 Origin of the orbitsphere

The charge distribution of the orbitsphere satisfies the condition of nonradiation. This means that the orbitsphere is stable in the sense that it does not lose energy by radiation. This condition is given by Haus [52] and is based on the classical Maxwell equations. The application of this condition to the orbitsphere is derived by Mills [45], but is missing in other articles. We have not extensively checked this derivation.

Mills does not just postulate the charge distribution (equations (A.3) and (A.4)), but claims that the equations are solutions of a wave equation in three dimensions plus time,

$$\left( \nabla^2 - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \right) \rho(r, \theta, \phi, t) = 0,$$

(A.5)

where $\rho(r, \theta, \phi, t)$ is the charge distribution and $\nabla^2$ is the Laplacian in spherical coordinates. This wave equation appears in published articles [43, 44] and in the October 2007 edition of the book [45], equation (1.1).

There are two problems with the wave equation. First it is unclear where this wave equation comes from. It seems to be postulated, but no proper explanation is given.
A.4 Conclusion

why. Secondly, and more importantly, the derivation is incorrect, as noted by Rathke\textsuperscript{4} \cite{Rathke}. The proposed distributions are no solutions of the wave equation.

Rathke also notes that the wave equation is not Lorentz invariant for velocities $v$ other than the speed of light $c$. A theory based on this equation can thus at best be a non-relativistic approximation. Mills says in a response \cite{MillsResponse} that although the equation is not Lorentz invariant, the solution of the two dimensional wave equation on a spherical shell is.

Mills changed the first chapter of his book \cite{Mills} in the June 2008 edition\textsuperscript{5}. Instead of the wave equation he takes on a different starting point: a generalized expansion of vector spherical waves, as given by Jackson \cite{Jackson}. The wave equation still appears later on in the text, as equation (1.56). We have not extensively checked this new approach, and no published comments exist on the June 2008 edition of the book.

\textbf{A.4 Conclusion}

The interesting question is if hydrinos exist. If Mills is right with his GUToCP, this means a revolution in theoretical physics. If he is wrong there might be a small chance that relativistic quantum mechanics would allow a hydrino state of hydrogen. But in the latter case the properties of hydrinos and the way they are produced are most likely very different than described by Mills.

The hydrino theory is described by Mills in his book \cite{Mills}, and all the published articles ultimately refer to this book. The book is not peer reviewed, and no articles have been published that comment on the newest edition (June 2008).

\textbf{A.4.1 Experiments}

The experimental results of Mills are a different matter. More debate is going on in the scientific world about the experiments than about the theory. There are three types of experiments involving plasma physics that—according to Mills—could confirm the existence of hydrinos. The first and most convincing would be the finding of excess energy in the calorimetric experiments, but this has not been reproduced independently by others than Mills et al. Secondly there is excessive line broadening. This has been reproduced by several independent groups, including ours. But there is much debate going on about the cause of the broadening. And thirdly the results in EUV spectroscopy. These have been partially reproduced in this thesis. In this case too there are many uncertainties about the exact interpretation of the results.

\textsuperscript{4}Rathke’s comment is sloppy and contains errors, although this does not affect the conclusion.

\textsuperscript{5}The June 2008 edition of \cite{Mills} is an online version which is continuously updated. The last update at the time of writing is from March 19, 2009.
Appendix B

Fourier optics

In this appendix we will give some general theory about a very convenient way to describe an optical system. It will be shown that under certain conditions an approximation can be applied in which the diffraction pattern can be described by the Fourier transform. Also some useful properties of the Fourier transform are given, that are used in section 3.2.

B.1 Field approximations

Light is an electromagnetical wave. It can be fully described by the electric field (and consequently the magnetic field). This means that the behavior of light is ultimately governed by the Maxwell equations (see also [32]). The mathematics involved in calculating diffraction effects can however be very complicated, and often there is no exact solution. Luckily this is not as bad as it may seem, since most of the time we are not interested in knowing the electric field everywhere. It is sufficient to know the field only at specific locations, for example the location of a screen. This allows us to use approximations.

Let’s look at the general case, where an aperture\(^1\) diffracts light that falls on a screen a distance \(R\) away. \(D\) is a characteristic size of the diffracting aperture, and \(\lambda\) is the wavelength of the light. The first assumption is that we look at distances many wavelengths from the aperture, \(R \gg \lambda\). In this region it is sufficient to use a scalar diffraction theory, which is a considerable simplification compared to vector theory needed when boundaries of the aperture are approached to within a few wavelengths. But scalar diffraction theory still is mathematically complex. To introduce further approximations it is useful to introduce the Fresnel number. It is a dimensionless measure for different optical regimes, and is defined as

\[
N = \frac{D^2}{\lambda R}
\] (B.1)

\(^1\)The term aperture can be taken in the general sense, which means any shape that transmits or reflects light. Other appropriate terms would be filter or grating.
When the Fresnel number is large, \( N \geq 1 \), an approximation known as \textit{Fresnel diffraction} applies. Because this approximation is valid close (but not too close) to the aperture, it is also called the \textit{near-field approximation}.

An approximation that simplifies the calculations even more is \textit{Fraunhofer diffraction}. Fraunhofer diffraction is valid far away from the aperture, when \( N \ll 1 \), and therefore known as the \textit{far-field approximation}. The most apparent approximation in Fraunhofer diffraction is that the curvature of the wavefront is neglected. When a spherical wavefront is viewed from far enough, it can be considered plane. This means that when the viewing distance \( R \) changes, the size of the diffraction pattern changes uniformly. The shape stays the same.

Fresnel diffraction does include the wavefront curvature, and is thus more complex. However, in the near-field diffraction effects are usually limited to the edges of a shape. In this region geometrical optics will be a pretty good approximation.

The far-field can actually be quite far. When an aperture with size \( D \) is 1 cm is illuminated with a wavelength \( \lambda \) of 400 nm, the Fraunhofer regime is at distance \( R \gg 250 \) m. However, the Fraunhofer diffraction pattern can made visible at much closer distances by using a lens. By putting a positive lens with a screen in its focus point, the plane wavefronts in the diffraction pattern are focussed on the screen, and this plane wavefront are exactly the parts that make the Fraunhofer diffraction pattern. This will turn out to be useful.

### B.2 Fourier transformation

When a plane wavefront hits a screen at a normal angle, all parts hit the screen simultaneously. The phase across the screen is constant. When the wavefront falls in under an angle \( \theta \), the phase across the screen is not constant, but varies harmonically. The spatial frequency \( f \) of this variation is given by

\[
\sin \theta = f \lambda
\]  

The angle of an incoming plane wave can be associated with the frequency of the phase variation. This argumentation works the other way around. Similarly, if the phase variation across an aperture is harmonic, the frequency can be associated with the angle of an outgoing plane wave (see figure B.1). Moreover, a superposition of harmonic phase variations across an aperture can be associated with several plane waves going out under different angles. And—even better—according to Fourier theory \textit{any} phase variation can be expressed as a superposition of harmonic variations. This means that any aperture can be characterized by a series of outgoing plane waves under different angles.

This plane waves can be made visible, either by putting a screen far away, so the plane waves do not overlap, or by putting a lens with a screen in its focal point in front of the aperture. This is exactly the situation in the Fraunhofer regime. The different angles hit the screen at different spots and form a Fraunhofer diffraction

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The relation between the angle of the plane wave $\theta$ and the position $\xi$ on the screen is

$$\tan \theta = \frac{\xi}{R} \quad (B.3)$$

If $R \gg \xi$ the angle $\theta$ is small and $\tan \theta \approx \sin \theta$. The relation between the Fourier component with frequency $f$ and the position $\xi$ in the diffraction pattern is thus

$$f = \frac{\xi}{R \lambda} \quad (B.4)$$

This brings us to a very important conclusion, and that is that the Fraunhofer diffraction pattern of an aperture can be described by the Fourier transform of that aperture. The Fourier transform of a function $g(x)$ is defined as

$$\mathcal{F}\{g(x)\} = G(f) = \int_{-\infty}^{\infty} g(x) e^{-i2\pi f x} \, dx \quad (B.5)$$

We take $u(x)$ as the complex amplitude of the scalar field at the aperture, and $U(\xi)$ the complex amplitude at the screen. The Fraunhofer diffraction equation is

$$U(\xi) = C \int_{-\infty}^{\infty} u(x) e^{-i2\pi \xi x} \, dx \quad (B.6)$$

Aside from a constant phase factor $C$ preceding the integral, this expression is the Fourier transform of the aperture distribution, evaluated at frequency $f = \xi/R\lambda$. In

---

2It might look as though we have mixed up phase and amplitude. But phase and amplitude can be combined in the complex amplitude. And indeed the Fourier transform can be applied to apertures which block the light partially (changing the amplitude), and to phase gratings, or any combination.
general the Fourier transform must be done in two dimensions ($x$ and $y$), but for us the one-dimensional case is sufficient.

A detector however measures not the amplitude, but the intensity of the light. The intensity $I$ that is measured by a detector is follows

$$ I \sim U^2 $$

The actual relation depends on many external factors, like the sensitivity of the detector. This is out of the scope of this chapter, and moreover the absolute intensity is of less importance.

### B.3 Properties of Fourier transformation

With the Fourier transform a very powerful mathematical tool comes to our disposal. The transform has some very useful properties, which we shall present here without proof. Let $g(x)$ and $h(x)$ be two functions with their Fourier transform $G(f)$ and $H(f)$, and $a$ and $b$ two constants.

**Linearity theorem.** The transform of a weighted sum of functions is the weighted sum of their individual transforms.

$$ \mathcal{F}\{ag + bh\} = aG + bH \quad (B.8) $$

**Similarity theorem.** A stretch in the coordinates in the space domain results in a contraction in the frequency domain, plus an overall change in amplitude.

$$ \mathcal{F}\{g(ax)\} = \frac{1}{|a|} G\left(\frac{f}{a}\right) \quad (B.9) $$

**Shift theorem.** A translation in the space domain results in a linear phase shift in the frequency domain.

$$ \mathcal{F}\{g(x - a)\} = G(f) e^{-2\pi ifa} \quad (B.10) $$

**Convolution theorem.** Convolution of two functions in the space domain is equivalent to multiplication in the frequency domain.

$$ \mathcal{F}\{g(x) \otimes h(x)\} = \mathcal{F}\left\{ \int_{-\infty}^{\infty} g(u) h(x - u) du \right\} = G(f) \cdot H(f) \quad (B.11) $$

The opposite holds as well. Multiplication in the space domain is equivalent to convolution in the frequency domain.

$$ \mathcal{F}\{g(x) \cdot h(x)\} = G(f) \otimes H(f) \quad (B.12) $$

**Dual theorem.** When the transform of a function is transformed again, the original function is recovered, with the only difference that it is mirrored.

$$ \mathcal{F}\{G(f)\} = g(-x) \quad (B.13) $$

If the original function is even, the result after transforming twice is unchanged.
B.4 Some functions and their transforms

In the following we will present some useful mathematical functions and their Fourier transform. A nice graphical overview is given in [54].

**Delta function.** The Dirac delta function $\delta(x)$ has value 0 anywhere, except at $x = 0$ where the value is $\infty$ in such a way that the integral is 1. The transform is

$$\mathcal{F}\{\delta(x)\} = 1 \quad \text{(B.14)}$$

which means that the diffraction pattern of a point source is a constant function.

**Linear phase function.** A function with a linear phase change and constant amplitude has the transform

$$\mathcal{F}\{e^{2\pi i ax}\} = \delta(f - a) \quad \text{(B.15)}$$

The Dirac delta function described above is a special case ($a = 0$) of the dual of this rule.

**Rectangular function.** The rectangle function $\Pi(x)$ has value 1 if $|x| \leq \frac{1}{2}$ and 0 otherwise. Its transform is

$$\mathcal{F}\{\Pi(x)\} = \text{sinc}(f) \quad \text{(B.16)}$$

where the sinc function is defined as

$$\text{sinc}(x) = \frac{\sin(\pi x)}{\pi x} \quad \text{(B.17)}$$

This is the classical example of single slit diffraction.

**Two delta functions.** Two Dirac delta functions positioned at $\pm a$ have transform

$$\mathcal{F}\{\delta(x - a) + \delta(x + a)\} = 2 \cos(2\pi af) \quad \text{(B.18)}$$

This is the classical example of a double slit. The dual of this rule implies that the transforming a cosinus results in two delta functions.

$$\mathcal{F}\{\cos(2\pi x)\} = \frac{\delta(f - 1) + \delta(f + 1)}{2} \quad \text{(B.19)}$$

**Comb function.** The Dirac comb function is a set of delta functions defined as

$$\text{comb}(x) = \sum_{m=\infty}^{\infty} \delta(x - m) \quad \text{(B.20)}$$

Its transform is very conveniently similar to the original function.

$$\mathcal{F}\{\text{comb}(ax)\} = \frac{1}{|a|} \text{comb}\left(\frac{f}{a}\right) \quad \text{(B.21)}$$
B.5 An example

Here we will give an example of how Fourier optics can conveniently describe a diffraction grating. The requirement is that Fraunhofer diffraction is valid. This means that the diffraction pattern must be either focussed, or viewed far away.

The ideal grating has an harmonic amplitude distribution \( u(x) \). According to (B.6) and (B.19) the resulting Fraunhofer diffraction pattern \( U(\xi) \) is

\[
  u(x) = \cos\left(\frac{2\pi x}{d}\right) \quad \rightarrow \quad U(\xi) = C \left( \delta\left(\frac{\xi}{R\lambda} + \frac{1}{d}\right) + \delta\left(\frac{\xi}{R\lambda} - \frac{1}{d}\right) \right) \tag{B.22}
\]

with \( d \) the grating constant and \( R \) the distance between the grating and the location where the diffraction pattern is observed. The diffraction pattern consists of only two orders \( m = +1 \) and \( m = -1 \). The peaks are perfectly focussed and the position of the first order \( \xi_{+1} \) is proportional to the wavelength.

\[
  \xi_{+1} = \frac{R\lambda}{d} \tag{B.23}
\]

An interesting conclusion is that an harmonically varying amplitude distribution produces no higher orders. However a high quality grating with gradually varying amplitude distribution is difficult to manufacture. Most high quality gratings are made the old-fashioned way, and that is by carving a pattern in a grating with a sharp diamond tip.
Bibliography


[42] Private communication with J.J.A.M. van der Mullen.


