

Czech Technical University in Prague

Faculty of Mechanical Engineering

Bachelor Thesis



**ČESKÉ
VYSOKÉ
UČENÍ
TECHNICKÉ
V PRAZE**

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2019/2020

BACHELOR'S THESIS ASSIGNMENT

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 Study program: **Theoretical Fundamentals of Mechanical Engineering**
 Branch of study: **No Special Fields of Study**

II. Bachelor's thesis details

Bachelor's thesis title in English:

Spectrometric attachment

Bachelor's thesis title in Czech:

Spektrometrická předsádka

Guidelines:

Review the principles of existing mobile spectrometers, their characteristics and possible applications.
 Design the optical part of a spectrometer attachable to a mobile phone.
 Analyze the influence of each element to the spectral resolution of the device.
 Design the mechanical attachment.
 Make experiments with the designed spectrometer, find a way how to calibrate the wavelengths and how to process the pictures taken.

Bibliography / sources:

Hutley M.C.: Diffraction Gratings, Academic Press, 1982, ISBN 0-12-362980-2
 Nagibina I.M., Prokofjev V.K.: Spektralnye pribory i tehnika spektroskopii, Izdatel'stvo Mašinostroenie, Leningrad 1967
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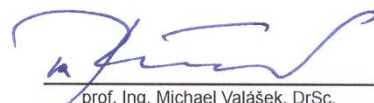
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Date of bachelor's thesis assignment: **31.10.2019** Deadline for bachelor thesis submission: **17.01.2020**

Assignment valid until: _____


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III. Assignment receipt

The student acknowledges that the bachelor's thesis is an individual work. The student must produce his thesis without the assistance of others, with the exception of provided consultations. Within the bachelor's thesis, the author must state the names of consultants and include a list of references.

 Date of assignment receipt


 Student's signature

Statement

I declare that I have worked out this thesis independently assuming that the results of the thesis can also be used at the discretion of the supervisor of the thesis as its co-author. I also agree with the potential publication of the results of the thesis or of its substantial part, provided I will be listed as the co-author.

Prague

Signature

Construction of the spectrometer

Abstract

The goal of the experiment was to construct a mobile spectrometer with high resolving power.

In the introduction part it was discussed why spectrometry is an important field of study and spectrometers might be useful in different areas of life.

The research was conducted in order to explain how spectrometry works from the optical point of view, and to calculate all necessary dimensions to create a device that would attach to the mobile phone with the camera.

The design was made so that the device would be as small as possible with the sufficient precision. The desired resolving power was chosen to be 0.6 nm, but due to limited resources, the resolving power appeared to be 1.887 nm.

After the design was completed and it was tested, the calibration was conducted to determine if the constructed spectrometer works correctly.

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List of symbols

λ – wavelength [nm]

T – temperature [K]

b – Wien's displacement constant [m*K]

c – speed of light [m/s]

k – Boltzmann's constant [J/K]

h – Planck's constant [J/s]

E – energy [J]

f – frequency [Hz]

d – slit width in diffraction grating [m]

φ, θ, ψ – symbols for angles [°]

j – order of diffraction [-]

m – order of interference [-]

D – angular dispersion

f' – focal length [mm]

pix – pixel size [μ]

M – magnification [-]

S – the width of the entrance slit of the spectrometer

l – length [mm]

RP – resolving power [nm]

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Introduction

Spectroscopy is a study of emission and absorption of light and other radiation by a matter. [1] The purpose of spectroscopy is to distinguish matter's qualities by the wavelength of radiation which is shown on the received spectrum. Spectroscopy has a variety of uses both in the science industry and in everyday life and it has a potential to be used even more. [2]

Every substance or object radiate and absorb light of different frequencies and wavelengths. Using this principle, scientists can analyze unknown substances and materials using spectrometers by comparing the results to known patterns in order to determine the composition of the tested sample.

Most spectrometers have three basic functions: they collect light (radiation), disperse the light into a spectrum and measure the intensities of lines produced from the. These lines are related to wavelengths.

Astronomers can use spectrometers to determine the composition of any new discoveries they make both on Earth and in distant galaxies. Also, the use of spectrometry in the medical field is growing in popularity as it can be used to identify contaminants or levels of various substances in the bloodstream to detect possible diseases or unwanted toxins. That might be very helpful as current methods would require taking at least 100 μ l of blood from a human vein. [3]

One more use for simple spectrometers could be determining the spectra of light sources for home. Not all colors of light have the same effect on human body. Blue wavelengths are beneficial during daylight hours as they boost attention, reaction times, and mood, but they are disruptive at night. The increasing amount in everyday life of electronics with screens, as well as energy-efficient lighting, is increasing people exposure to blue wavelengths, especially after sundown. [4] Some studies suggest a link between exposure to light at night, such as working the night shift, to several serious types of deceases such as cancer, diabetes, heart disease, and obesity. There is no strong proven correlation between nighttime light and conditions listed above. But it is scientifically proven that exposure to light - especially blue light - suppresses the secretion of melatonin, a hormone that influences circadian rhythms, and there is an experimental evidence that lower melatonin levels might explain the association with cancer.

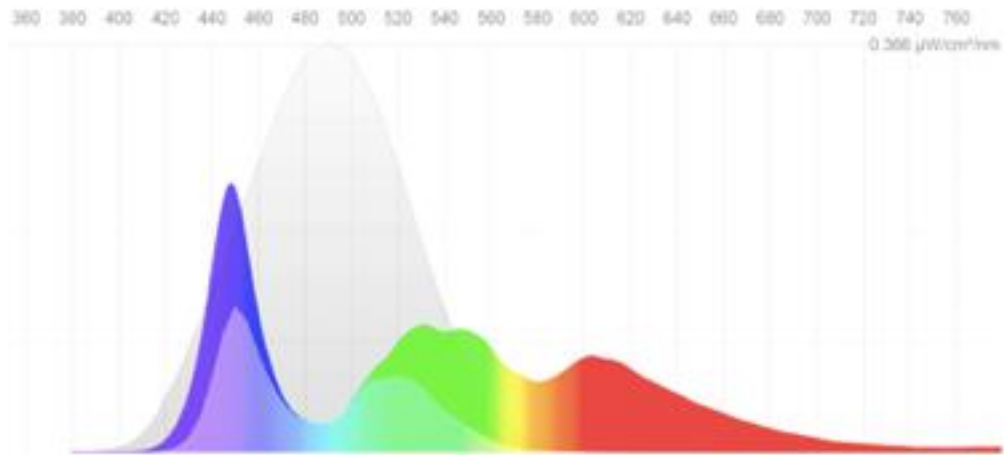


Figure 1 – iPhone 6 (2014 – year of the release) spectrum [5]

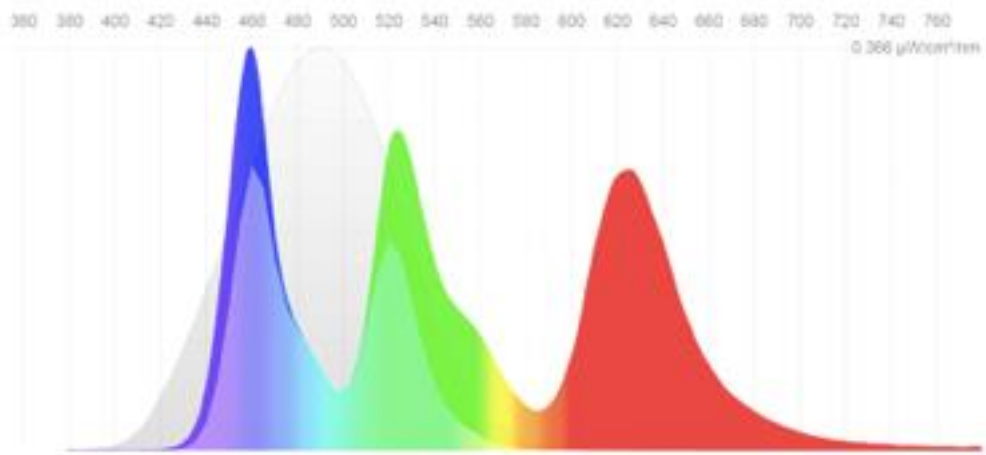


Figure 2 – iPhone X (2017 – year of the release) spectrum [5]

The two pictures above show examples of spectrums of two mobile phones: iPhone 6 (2014) and iPhone X (2017) respectively. The grey region on the pictures show which wavelengths are recognized by the human eye as the 'daytime' light, therefore increasing alertness and cognitive functions. The graphs also indicate that manufacturers try to increase the amount of blue light radiated from the phone screen. [5]

In order to determine the amount of blue light emitted from the light source spectrometer can be used.

Spectroscopy can be highly useful when it comes to medicine, especially pharmacy. Most of the pharmaceutical companies have already been using different kinds of spectroscopy (mass spectroscopy, nuclear magnetic resonance spectroscopy, excitation spectroscopy etc.) for

a long time for drug analysis. The process is usually consisting of getting a spectrum from a sample and comparing it with the original. [6] There are several startups working on compact spectrometers that can help people with no medical education or special expensive equipment, to distinguish pills. Some of them claim that they can figure out what a specific pill's reflective signature is and then compare known pills to others, data for which would be stored in a smartphone app's database. So, people seeking for qualitative pills may be able to scan it in order to see how they match up with the original ones. [7] The reason it might be hugely important is that fake drugs have proven to be a growing problem: in 2018, Interpol reported that it seized 20.7 million counterfeit medications in an operation aimed at rounding up those sold by online pharmacies. This was more than twice as much as they seized two years earlier.

Some kinds of spectroscopy, such as near-infrared (NIR), are also well-suited to nondestructive analysis of bulk, high-moisture samples like fruit, fish, meat etc. While challenging to interpret and analyze, NIR spectroscopy probes the vibrational overtone absorption of chemical bonds and is sensitive to most chemical constituents in foods. The resulting spectrum is often overlapping and complex, demanding chemometric analysis to understand its meaning. [8]

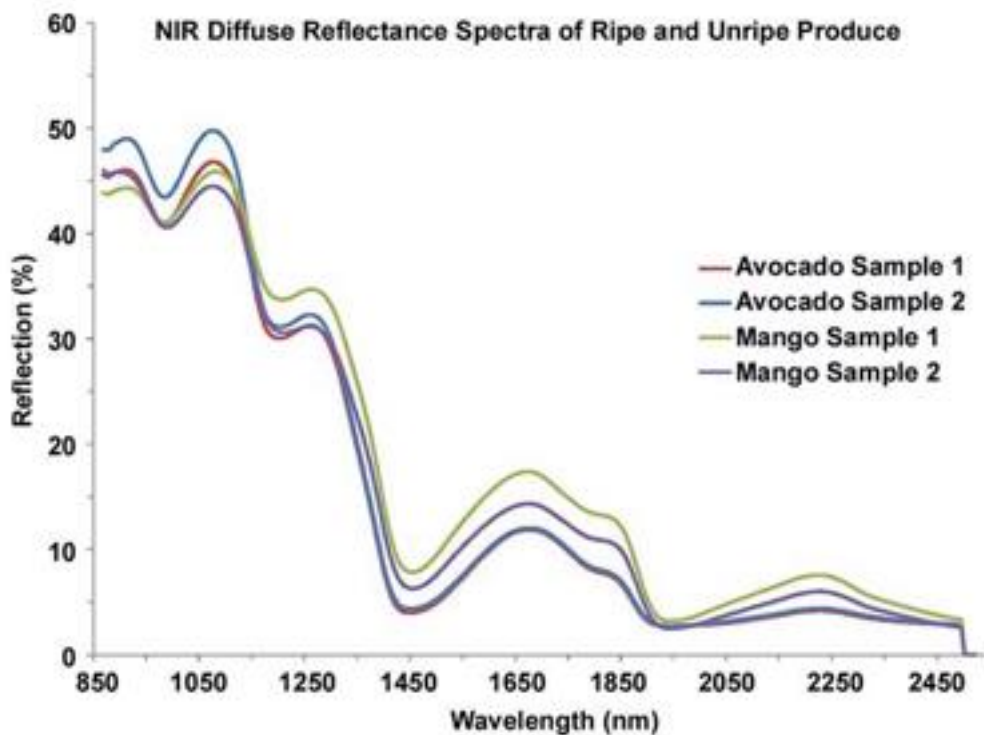


Figure 3 – spectrum of several food samples [9]

Light at NIR wavelengths penetrates deeply with less scattering, allowing internal composition to be analyzed via nondestructive reflectance and through-sample transmission techniques. When processed using a well-developed chemometric model, a simple NIR reflectance spectrum can be used to predict complex characteristics, such as an apple's ripeness, sweetness or storage duration.

Another - and probably the most noticeable - use of spectroscopy that affects humanity is astronomical spectroscopy. It is the study of astronomy using the techniques of spectroscopy to measure the spectrum of electromagnetic radiation, which radiates from celestial objects. A stellar spectrum can reveal a lot of properties of stars for example their chemical composition, temperature, density, mass, distance, luminosity etc. Spectroscopy is also used to study the properties of many other types of celestial objects such as planets, nebulae, galaxies, and active galactic nuclei. [10]

Research

Electromagnetic interactions

Electricity and magnetism were thought earlier in history to be separate forces. However, in 1873, Scottish physicist James Clerk Maxwell developed a theory of electromagnetism. The study of electromagnetism deals with how electrically charged particles interact with each other and with magnetic fields. [11]

There are four main electromagnetic interactions:

- The force - between electric charges - of attraction or repulsion. The value is inversely proportional to the square of the distance between them.
- Magnetic poles that come in pairs attract or repel each other like electric charges do.
- An electric current in a wire produces a magnetic field direction of which depends on the direction of the current.
- A moving electric field produces a magnetic field.

Bohr model of atom

Scientific ideas of an atom were always changing. Since the ancient times, an atom was usually thought to be a very small indivisible piece of matter that changes shape in order to change the properties of a substance. These concepts were then used in the John Dalton's theory in 1803. In 1897 J.J. Thomson have finally discovered electrons and in 1904 has created a theory which described atom as negatively charged electrons scattering throughout a spherical positively charged cloud. Ernest Rutherford in 1911 has found that the positive nucleus is located in the center of an atom and relatively small to the area where negative electrons are scattered. [12]

Bohr atomic model, description of the structure of atoms was proposed in 1913 by the Danish physicist Niels Bohr. [13] The Bohr model of the atom was the first that included quantum theory and was one of the predecessors of quantum-mechanical models. The Bohr model and all its successors describe the properties of atomic electrons in terms of a set of allowed, or possible, values. Atoms absorb or emit radiation only when the electrons quickly jump between

allowed, or stationary, states (levels). Direct experimental evidence for the existence of such discrete states was obtained in 1914 by the German physicists James Franck and Gustav Hertz.

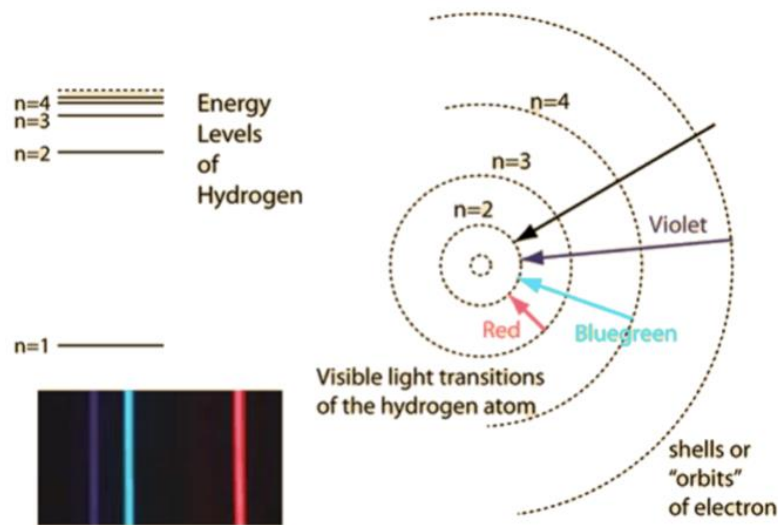


Figure 4 – Bohr's model of atom

The electrons in free atoms can only be found in certain discrete energy states. These sharp energy states are associated with the orbits of electrons in an atom. One of the implications of these quantized energy states is that only certain photon energies are allowed when electrons jump down from higher levels to lower levels, producing the hydrogen spectrum. The Bohr model successfully predicted the energies for the hydrogen atom but had significant failures that were corrected by solving the Schrodinger equation for the hydrogen atom. [14]

Waves

Electromagnetic radiation is created when an atomic particle, such as an electron, is accelerated by an electric field, causing it to move. [15] The movement produces oscillating electric and magnetic fields, which travel at right angles to each other in a bundle of light energy called a photon. Photons travel in harmonic waves at the fastest speed possible in the universe: 299,792,458 meters per second in a vacuum, also known as the speed of light.

The waves have certain characteristics, given as:

- frequency [Hz] - number of waves per unit of time;
- wavelength [m] - distance between two consecutive peaks;
- energy [J] - that is being transferred by a wave.

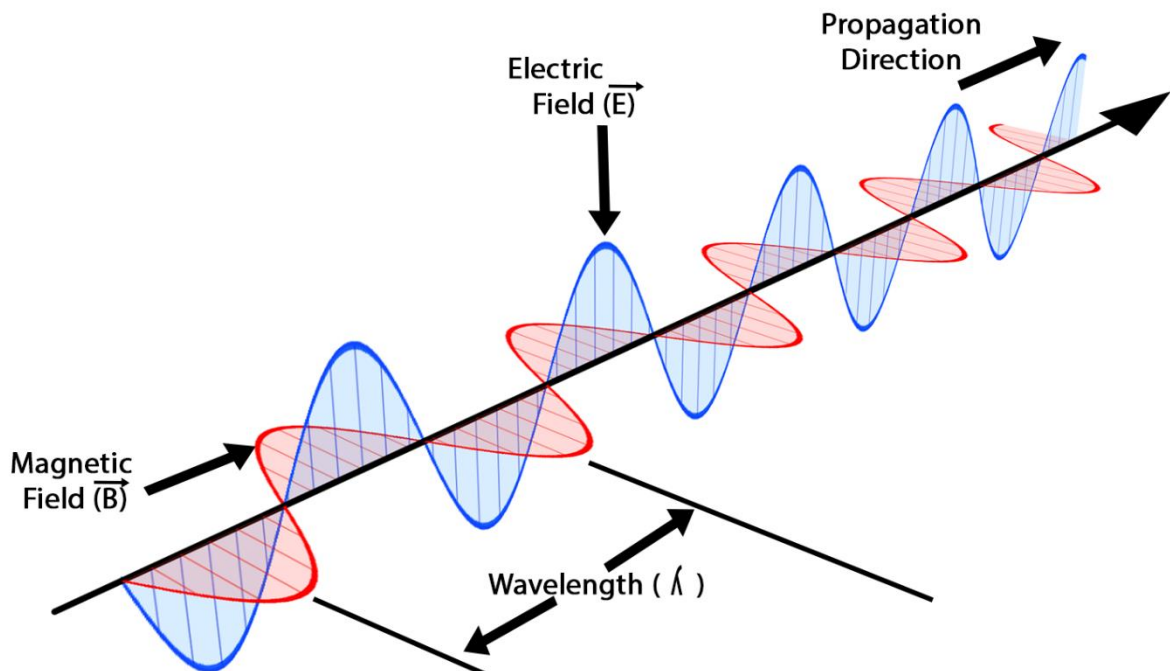


Figure 5 – electric and magnetic wave propagation [16]

Electromagnetic spectrum

The electromagnetic spectrum shows the distribution of the electromagnetic radiation and is generally divided into seven regions, in order of decreasing wavelength and increasing frequency. The common designations are listed in a table below. Nearly all frequencies and wavelengths of electromagnetic radiation can be used for spectroscopy. [17]

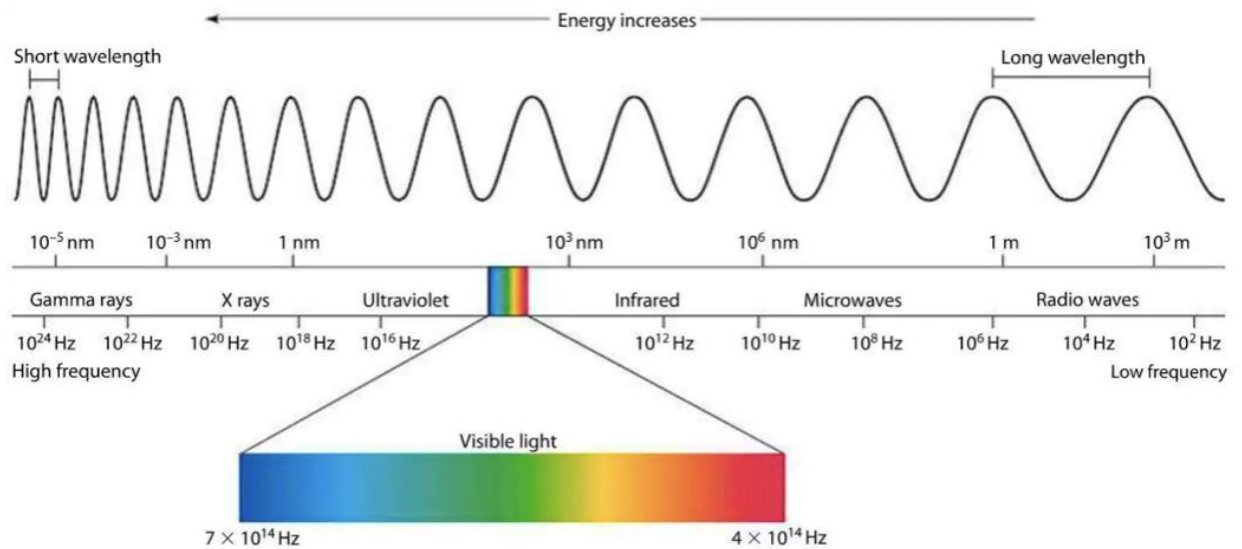


Figure 6 – electromagnetic spectrum [18]

Type of waves	Range of wavelengths [nm]	Range of frequencies [Hz]	Uses
Gamma rays	<1	>3*10 ¹⁷	Medical treatment, can kill bacteria and cancer cells etc.
X-rays	1-10	3*10 ¹⁶ -3*10 ¹⁷	Medical treatment, checking for broken bones, pneumonia, cancer etc.
Ultraviolet light	10-400	7.5*10 ¹⁴ -3*10 ¹⁶	Sterilization; detecting forged bank notes; production of vitamin D in human body etc.
Visible light	400-700	4.3*10 ¹⁴ -7.5*10 ¹⁴	Used by humans to observe the world
Infrared	700-10 ⁵	3*10 ¹² -4.3*10 ¹⁴	Thermal imaging cameras
Microwave	10 ⁵ -10 ⁸	3*10 ⁹ -3*10 ¹²	Cooking in microwave ovens
Radio wave	>10 ⁸	<3*10 ⁹	Communication

Table 1 – electromagnetic spectrum [19] [20-23]

Usually, lower-energy radiation, such as radio waves, is expressed as frequency; microwaves, infrared, visible and UV light are usually expressed as wavelength; and higher-energy radiation, such as X-rays and gamma rays, is expressed in terms of energy per photon. However, these characteristics are related to each other and can be described by the following formulas:

$$c = f * \lambda \quad [1]$$

$$E = h * f \quad [2]$$

where c is speed, f is frequency, λ is a wavelength, E is energy of the photon and h is a Planck's constant

Planck's Law

Newton used a prism to split white light into a spectrum of color. Fraunhofer's high-quality prisms allowed scientists to see dark lines of an unknown origin. In the 1850s, Gustav Kirchhoff and Robert Bunsen described the phenomena behind these dark lines. Hot solid objects produce light with a continuous spectrum, hot gases emit light at specific wavelengths, and hot solid objects surrounded by cooler gases show a near-continuous spectrum with dark lines corresponding to the emission lines of the gases. By comparing the absorption lines of the sun with emission spectra of known gases, the chemical composition of stars can be determined. The major Fraunhofer lines, and the elements with which they are associated, can be found in the specific table. [25]

In 1860 Gustav Kirchhoff proposed the idea of a black body, a material that emits electromagnetic radiation at all wavelengths. In 1894 Wilhelm Wien derived an expression relating the temperature of a black body to its peak emission wavelength.

$$\lambda_{max} * T = b \quad [3]$$

where b is a constant of proportionality called Wien's displacement constant, equal to $2.8977729 \times 10^{-3} \text{ m} \cdot \text{K}$. This equation is called Wien's Law. By measuring the peak wavelength of a star, the surface temperature can be determined.

In 1900 Max Planck combined classical principle of spectral-energy distribution of radiation with his assumption that energy is being radiated by certain amounts called quanta of energy. The amount of the energy radiated per unit volume can be described by the following formula: [24]

$$E = \frac{2\pi hc^2}{\lambda^5 (e^{\frac{hc}{\lambda kT}} - 1)} \quad [4]$$

where c is a speed of light equal to 299,792,458 m/s, k is Boltzmann's constant equal to $1.381 \times 10^{-23} \text{ J/K}$, h is Planck's constant equal to $6.626 \times 10^{-34} \text{ J/s}$.

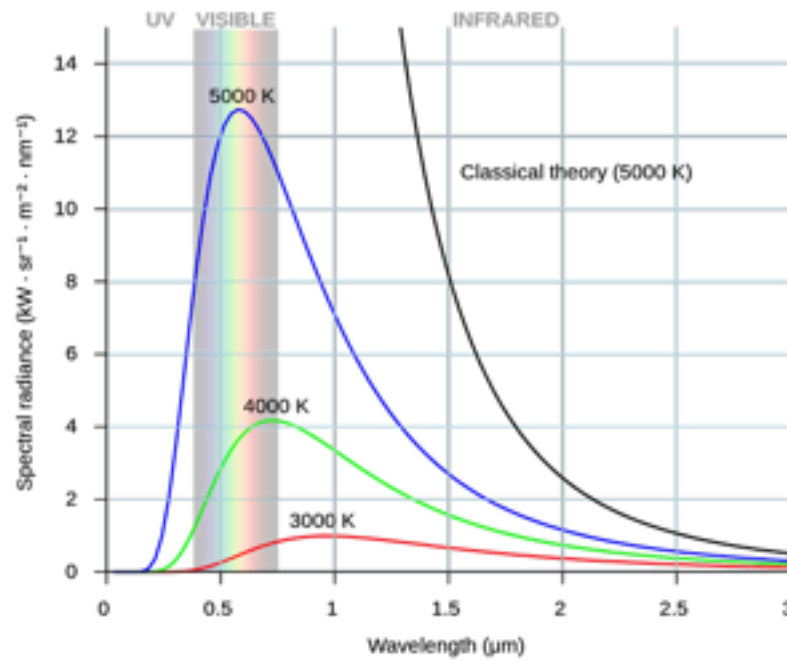


Figure 7 – Planck's law [25]

Propagation of Light

Propagation of light can be described by the following characteristics from geometrical optics: transmittance (passing of light through a medium), reflection (throwing back of a beam of light) and refraction (changing the angle of direction of the beam of light depending on the refractive index which is equal to the relation between the speed of light in vacuum and the speed of light in the given medium.) [26]

Propagation of light can also be described by the wave optics theory. Its characteristics - dispersion, diffraction and interference - will be more deeply described in the chapters below.

[27]

Dispersion

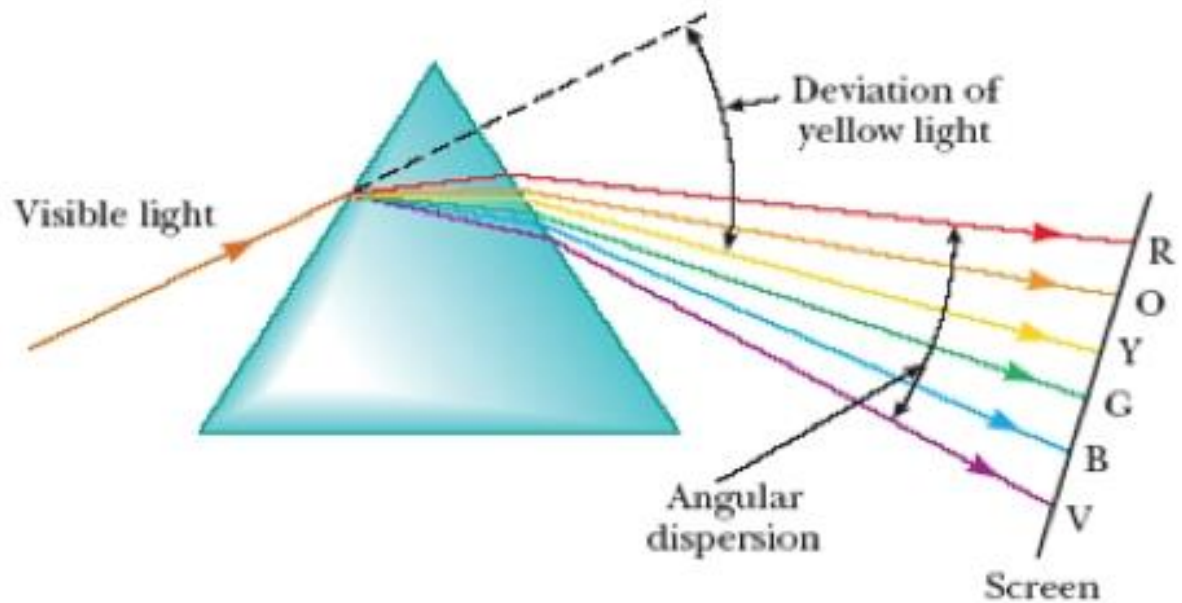


Figure 8 – demonstration of dispersion [28]

The method of dispersion used in spectroscopy is shown in the pictures above. Dispersion is the separation of light into a spectrum by refraction. The index of refraction is a function of wavelength

$$n = f(\lambda) \quad [5]$$

Refractive index is reversely proportional to the wavelength. The relation can be described by the Cauchy's formula:

$$n = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \dots \quad [6]$$

where A, B, C are constants.

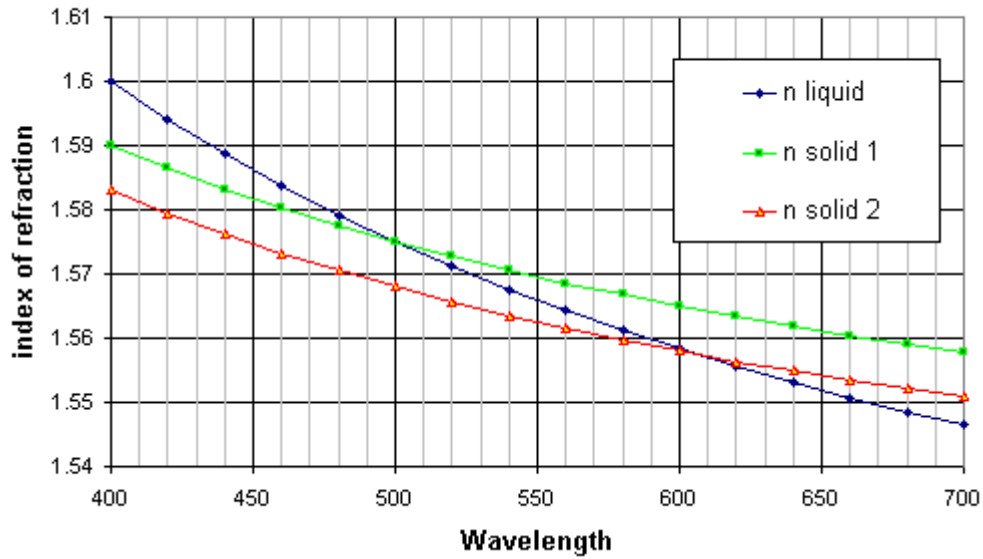


Figure 9 – graph of dependence of index of refraction on wavelength [29]

Dispersion prisms (one or several) can be used in spectroscopy instruments. Due to the refraction on the edges of prisms the beam of light is deviated by some angle θ to the original. The angle of deviation depends on the refraction index and therefore it is the function of wavelength

$$\theta = f(\lambda) \quad [7]$$

Interference

Interference is a phenomenon in which two or more waves superimpose with a formation of a resultant wave which has greater or lower amplitude. Therefore, interference can be constructive, or destructive. [38] The phenomenon is supported by the double-slit experiment conducted by Thomas Young. The pure-wavelength light was sent through two vertical slits in front of a screen. It resulted in a pattern of several vertical lines spread out horizontally. [39]

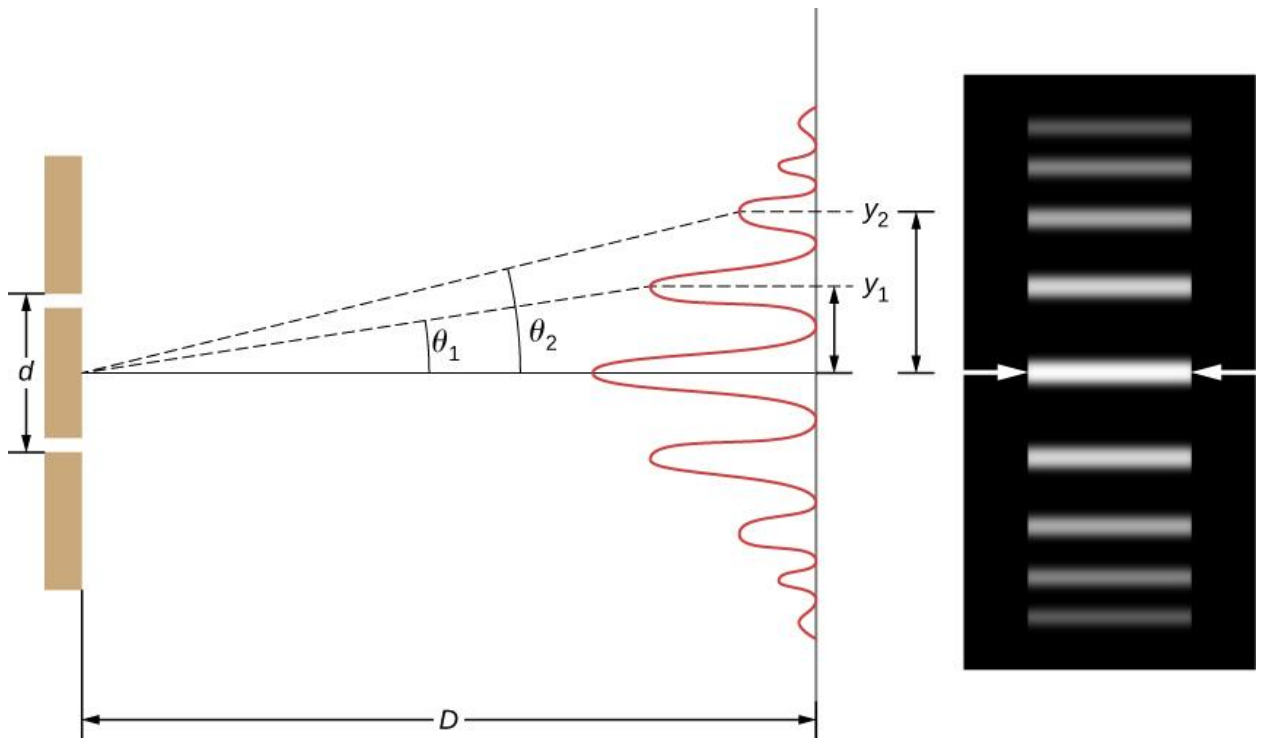


Figure 10 – Young's double-slit experiment

The picks on the screen are called orders of interference. The position of the peaks depends on the wavelength, distance between slits and distance between sources of waves and the screen.

$$y_n = \frac{m \cdot D \cdot \lambda}{d} \quad [8]$$

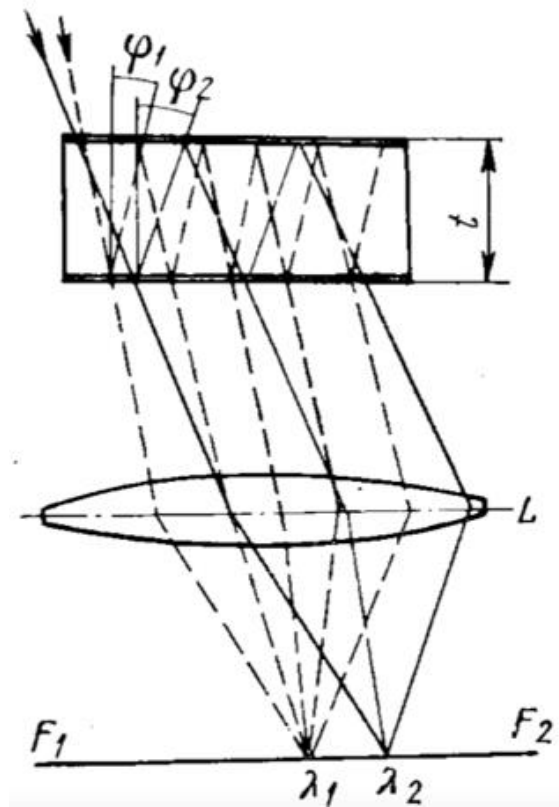


Figure 11 – principle of interference in spectrometers [27]

Interference in spectrometers can be described by the following equation:

$$2t * \cos\phi = m\lambda \quad [9]$$

where ϕ is an angle of incident ray and m is the order of interference.

Diffraction

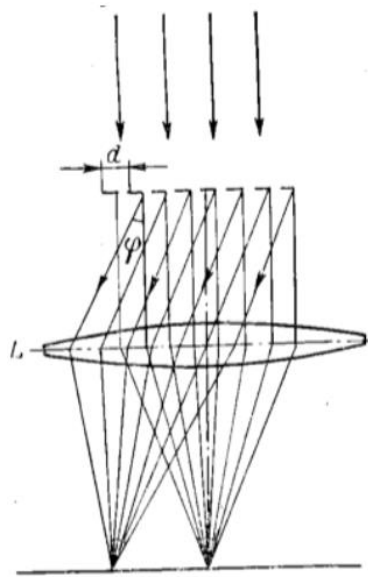


Figure 12 – principle of diffraction [27]

Diffraction is a phenomenon, that occurs when light either hits an obstacle or passes through a slit. In spectroscopy the process of diffraction of parallel beams of light from the big amount of same narrow slits called diffraction grating is used. The diffraction is a multiple interference of many beams therefore it would have sharp and narrow diffraction maxima related to the different angles of diffraction. The relation can be described by the following formula:

$$d(\sin\psi + \sin\varphi) = m\lambda \quad [10]$$

where φ is an angle of diffraction, m is the order of interference, d is the groove separation, called the grating constant, ψ is the angle of incident beam which is equal to therefore its \sin is also equal to zero, λ is the wavelength and m is an order of interference. [27]

Diffraction grating

Diffraction grating can either contain parallel slits of the same width or have parallel grooves from which the light beams would reflect. In my experiment the second type of diffraction gratings will be used.

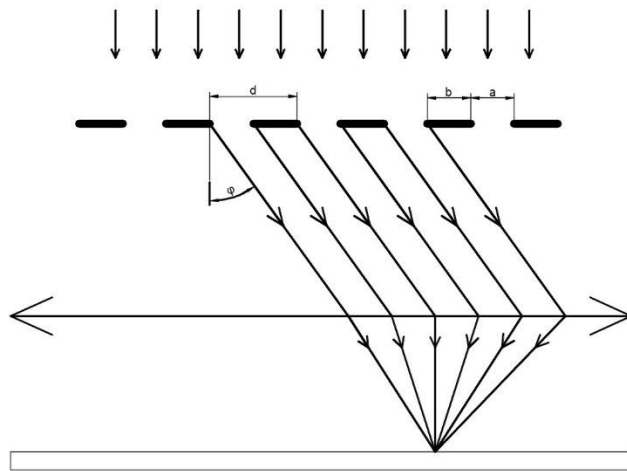


Figure 13 – principle of diffraction grating [30]

The higher the number of slits in the diffraction grating - the bright regions of the spectrum are narrower and brighter, while dark regions are darker. It is shown on the picture below:

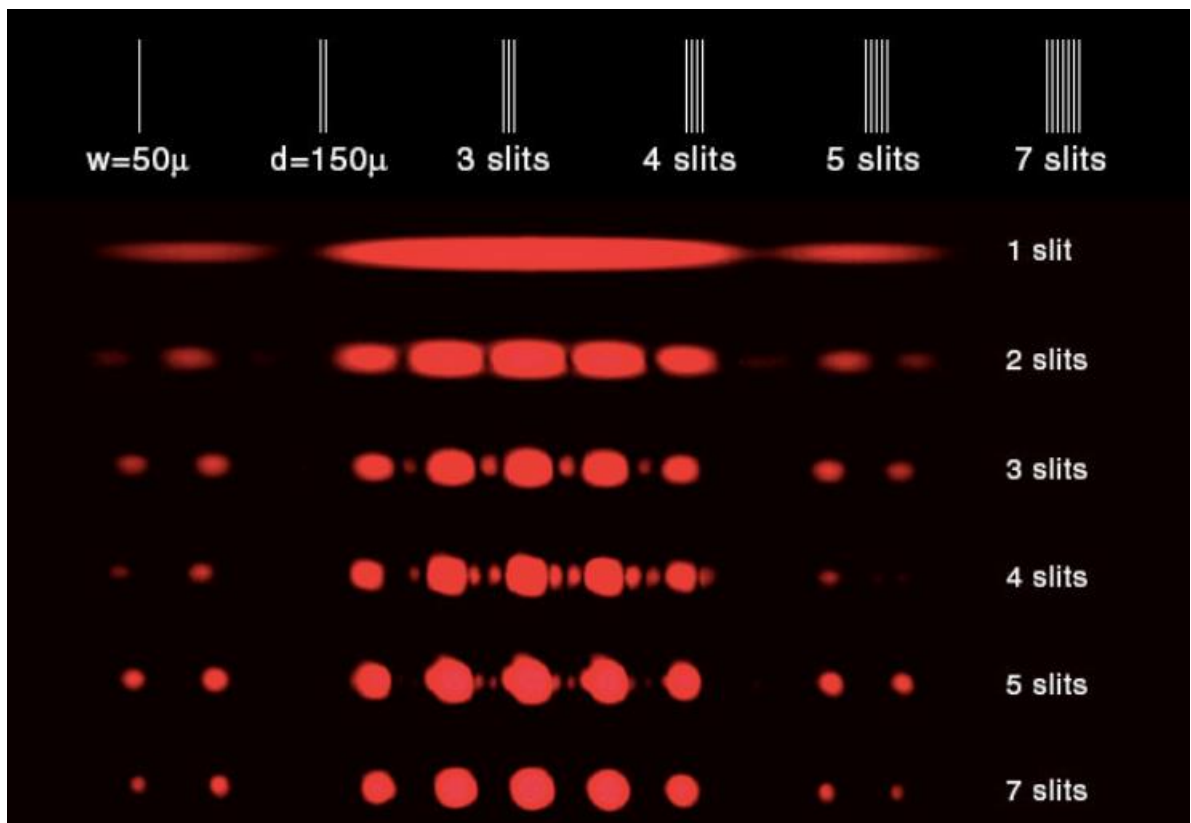


Figure 14 – comparison of different number of grooves in diffraction grating [31]

Condition of the maxima is described in equation 10.

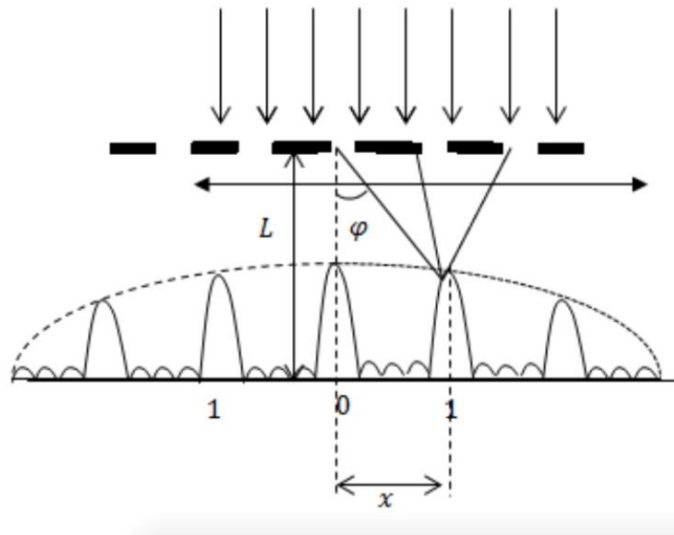


Figure 15 – distribution of orders in diffraction grating

The formula for the angular dispersion will be found by taking a derivative of equation 10:

$$\frac{d\phi}{d\lambda} = \frac{m}{d \cdot \cos\phi} \quad [11]$$

Spectrometer structure

According to a definition, spectrometer is a device for measuring wavelengths of light over a wide range of the electromagnetic spectrum. It is widely used for spectroscopic analysis of sample materials. [32]

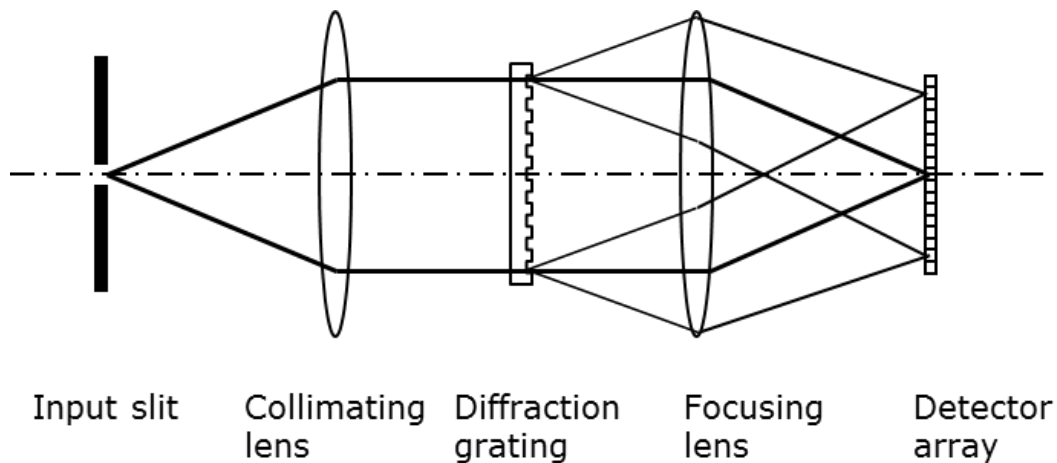


Figure 16 – schematic design of a spectrometer [40]

Firstly, the light is passing through an entrance slit, collimating lens (or several of them) is creating a focusing system with a parallel light beams, D is a diffraction grating, focusing lens focuses the light onto the detector.

The first step in the process is to receive beam of light through a narrow aperture called an entrance slit. In most spectrometers, it is then collimated by a lens and directed onto a grating. The grating then disperses the spectral components of the light at varying angles, which is then focused by a second lens and imaged onto the detector. [33]

Once the light is imaged onto the detector the photons are then converted into electrons which are digitized to a computer. The software then interpolates the signal based on the number of pixels in the detector and the linear dispersion of the diffraction grating to create a calibration that enables the data to be plotted as a function of wavelength over the given spectral range.

The formulas for determination of the dimensions of slit and focal lenses will be discussed later in the “Experiment” part.

Classification of spectroscopy

There are two types of spectra: absorption and emission. For the absorption spectra the incident light from the light source can be transmitted, absorbed or reflected through the sample. The changes occurred during the interaction of incident light with the sample reveals the sample characteristics. that holds for absorption spectra. There are also samples emitting radiation – light sources, for example stars – emission spectra are measured for such samples

Two types of radiation sources are generally used in spectrometer – continuous and line sources. Continuous sources are heated solid substances or lamps that emit light over a wide wavelength range, and line sources are specialized lamps and lasers.

Spectroscopy is a broad field that many sub-disciplines exist, each with several implementations of specific spectroscopic techniques. The various implementations and

techniques can be classified in several ways. [34] First of all, the types of spectroscopy are distinguished by the type of radiative energy involved in interaction. In many applications, the spectrum is determined by measuring changes in the intensity or frequency of this energy. The types of spectroscopy also can be distinguished by the nature of the interaction between the energy and the material. Spectroscopic studies are also classified by which specific type of matter radiant energy interacts with. The examples are: atomic, molecular, crystal and nuclear etc. Other types of spectroscopy are distinguished by specific applications or implementations.

Experiment

The goal of the experiment was to create a device – an attachment for a mobile phone with a camera – that could be used as a spectrometer. The resolving power of the device was required to be as good as possible with given conditions.

The experiment consisted of several parts:

- Research – finding all required formulas, camera specifications, as well as calculations of the dimensions required for the design;
- Design of the device – research of the devices that are similar to mobile spectrometers, finding the optimal design for the device, drawing the attachment in AutoCAD 3D;
- Assembly – printing of the device, finding suitable lens, making diffraction grating and the entrance slit, attaching the device to the mobile phone;
- Calibration – after the spectrometer is complete, it is used to distinguish the spectrum of the light of known spectrum to compare the results.

Research

The mobile phone used in the experiment was Apple iPhone SE, the list of the camera specifications required for the further calculations is below:

Image sensor	Sony IMX315 Exmor RS
Focal length	4.02 mm
Number of pixels	4032 x 3024
Pixel size	1.19 nm
f-number	2.2

Table 2 – camera specifications [37] [43]

Calculations

As it was discussed in the theory part of the thesis, the spectrometer contains of the entrance slit, collimator, diffraction grating, camera lens and the detector. The last two pieces are located inside the mobile phone.

The entrance slit would determine the amount of light coming into the spectrometer, therefore there should be enough light for the camera to detect it, but from the other side it should be small enough in order to distinguish the spectrum (the impact of the slit width to the spectrometer's resolving power will be explained later). Collimator lens forms a beam of parallel rays in a direction perpendicular to the diffraction grating, will be chosen to be with small diameter and short focal length, as the aim is to create device as compact as possible. The diffraction grating of a spectrometer is a crucial part of the device, it influences the spectrum width and the resolving power that the spectrometer will achieve. The grating will influence an optical resolution and the maximum efficiency for a specific wavelength range, but it is limited by the number of slits per unit of length.

Grating equation:

$$\sin\varphi + \sin\psi = \frac{m\lambda}{d} \quad [13]$$

where angle ψ is an angle of incident ray (design of the device will make this angle equal to 0, therefore \sin of this angle also will be equal to 0), m is an order and can be negative, for my experiment I will use only values of +1 and -1, d is the distance between two slits in the diffraction grating.

Formulas for angular and linear dispersion respectively:

$$D = \frac{d\varphi}{d\lambda} = \frac{m}{d \cdot \cos\varphi} \quad [14]$$

$$\frac{dl}{d\lambda} = \frac{1}{f'_{cam} D} \quad [15]$$

where D is the angular dispersion, and f'_{cam} is the focal length of camera – this value is given. This value shows how the beams of light of different wavelengths are separated.

Formula for magnification:

$$M = \frac{pix}{ES} = \frac{f'_{cam}}{f'_{lens}} \quad [16]$$

where ES is the width of the entrance slit, pix is the pixel size which is given by the manufacturer, f'_{lens} is the focal length of the lens.

Here is the scheme of the diffracted light passing through the focusing lens and reaching the detector inside the phone.

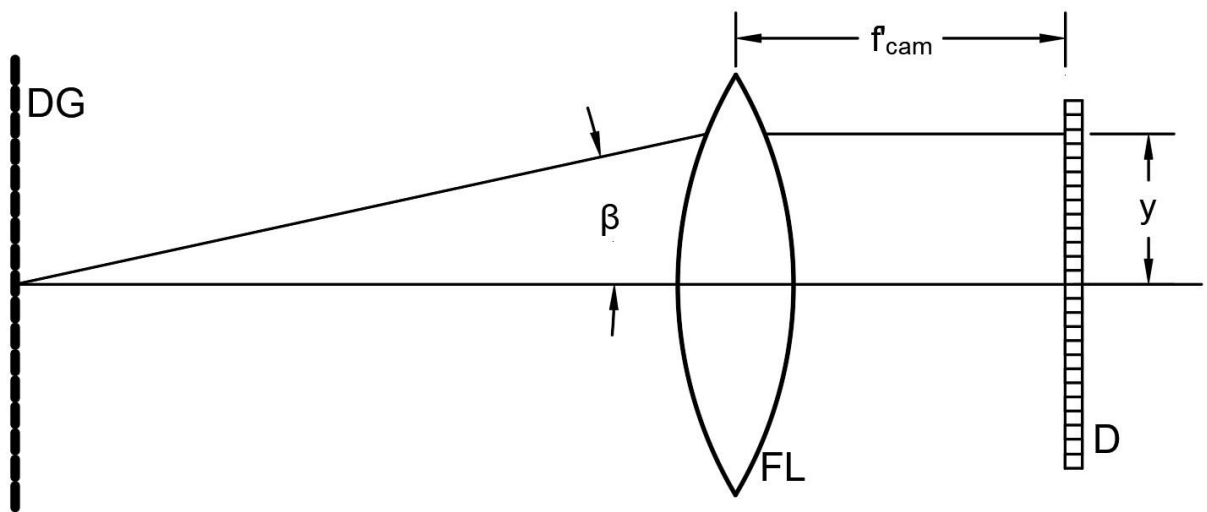


Figure 17 – scheme of light passing through the spectrometer

where: DG is the diffraction grating, β is the angle of diffraction, f'_{cam} is the focal length = of the focus lens (FL in the picture) the value of which was found before, D is the detector, and y is the distance between the axis and the place where the light of specific wavelength reaches the detector.

The resolving power is Δy_{λ} , the minimum difference between two spectral lines that are seen as separate lines.

From the figure 17 we see that:

$$RP = y_{\lambda_1} - y_{\lambda_2} \quad [17]$$

where RP is resolving power.

Also, from that figure and using trigonometry we get the following formula:

$$y_{\lambda_1} = \frac{l * \lambda_1}{d * \sqrt{1 - \frac{\lambda_1^2}{d^2}}} \quad [18]$$

Combining the equations [17] and [18] and substituting known values we get:

$$\frac{f'_{cam} * \lambda_2}{d * \sqrt{1 - \frac{\lambda_2^2}{d^2}}} - \frac{f'_{cam} * \lambda_1}{d * \sqrt{1 - \frac{\lambda_1^2}{d^2}}} = RP \quad [19]$$

The whole process of calculations of entrance slit in Matlab is shown in the attachment #4. After performing calculations, we find out that resolving power of 0.6 nm is impossible to get under given conditions, therefore resolving power of 2 nm is chosen and grating density of $1/293.97 \text{ mm}^{-1}$ (293.97 grooves per 1 mm) is calculated.

Design

After receiving all the necessary values for dimensions, it was possible to start creating the model of the attachment. 3D printing the model was the most obvious decision for getting the attachment. AutoCad 3D was chosen as a software for drawing the model.

The first question was how to attach the device to the mobile phone itself. To make the device mobile, it was decided to attach it not to the phone but to the cover, so the spectrometer would be attached to the cover with the whole area of the back part of the cover. Picture of it is in the attachment #1.

The main problem faced was how to fit all parts of the spectrometer into one holder. It was decided to make two parts: first – the main piece that will hold all the parts of the spectrometer, and second part – the piece that will be attached to the main part by four bolts and nuts. The picture of the upper part is in the attachment #2.

Before talking about further details of the device it is necessary to mention that working with provided 3D printer was challenging as it was not precisely following the dimensions of those

made in the software. Therefore, for lens holder and grating holders it was important to conduct extra experiments to find out real gap for the holder.

The dimensions for the holders for the lens and the grating were chosen according to the dimensions of the grating and the lens themselves. So that, as the radius of the collimating lens is 20 mm the holder would be also with the radius of 20 mm, and the size of the grating holder also would be the same as the diffraction grating.

The next piece of the main part is the long tube, which dimension is chosen so that between the collimating lens and the slit would be the distance of the lens' focal length. This part is the largest in the device due to the value of the focal length.

The final part of the device is the entrance slit, calculation of width of which was described in the above chapter of the thesis from the two pieces of the broken razor blade glued to the edge of the tube. The reason is that we need sharp straight edges of the slit as the spectrum is monochromatic images of the slit. Any irregularities of the slit will be seen in the spectrum as deformations of the spectral lines. The picture of the whole spectrometer is in the attachment #3

Collimating lens

The collimating lens was pre-calculated according to the desired resolution and given parameters of the camera. The diameter of the chosen lens is 20 mm. The focal length of the lens was measured to be approximately 100 mm. In order to get the accurate value, the Cornu's method of measuring focal length was conducted, using a collimator and a microscope on an optical bench. The experiment was conducted twice with different orientations of lens.

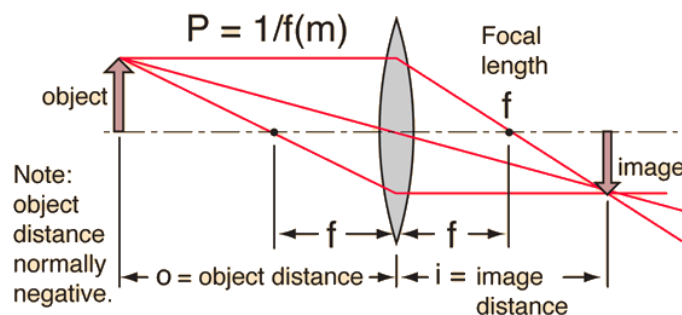


Figure 18 – the Newtonian form of lens equation [42]

The Newtonian form of the lens equation is the following:

$$f'^2 = |x * x'| \quad [20]$$

where x and x' are the distances between focus and the vertexes of the lens. The lens vertexes were used as the objects.

As the experiment was conducted twice the following values were obtained: 103.53 mm and 105.54 mm. The first value was chosen as this orientation was used in the final design of the spectrometer.

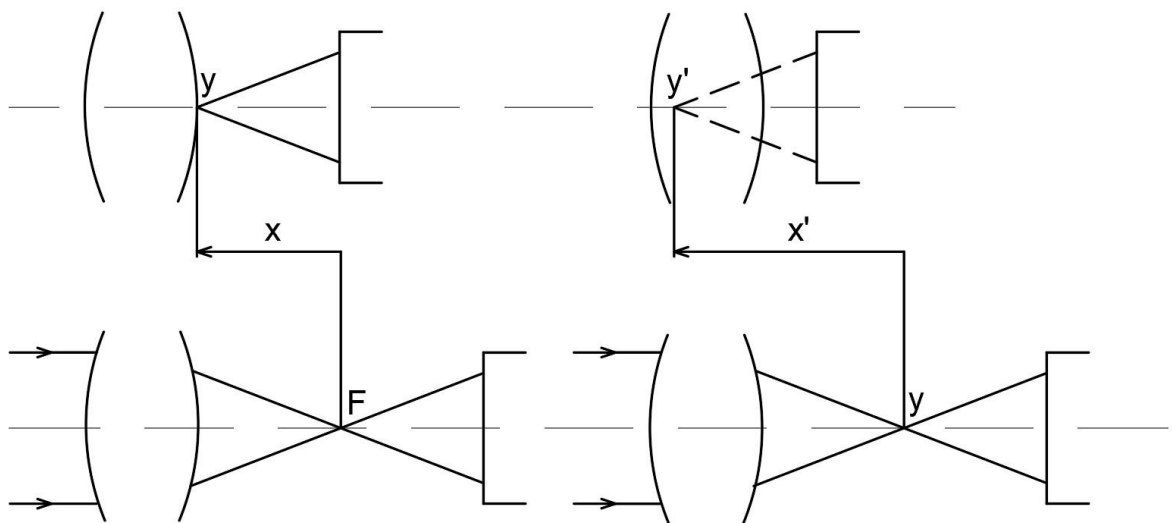


Figure 19 – focal length determination experiment

As the value of the focal length is known, now it is possible to calculate the required width of the entrance slit. After solving the equation [16] the width of the entrance slit must be 44.09 μm .

Diffraction grating

The next step of the experiment was to create a diffraction grating with the desired grating density.

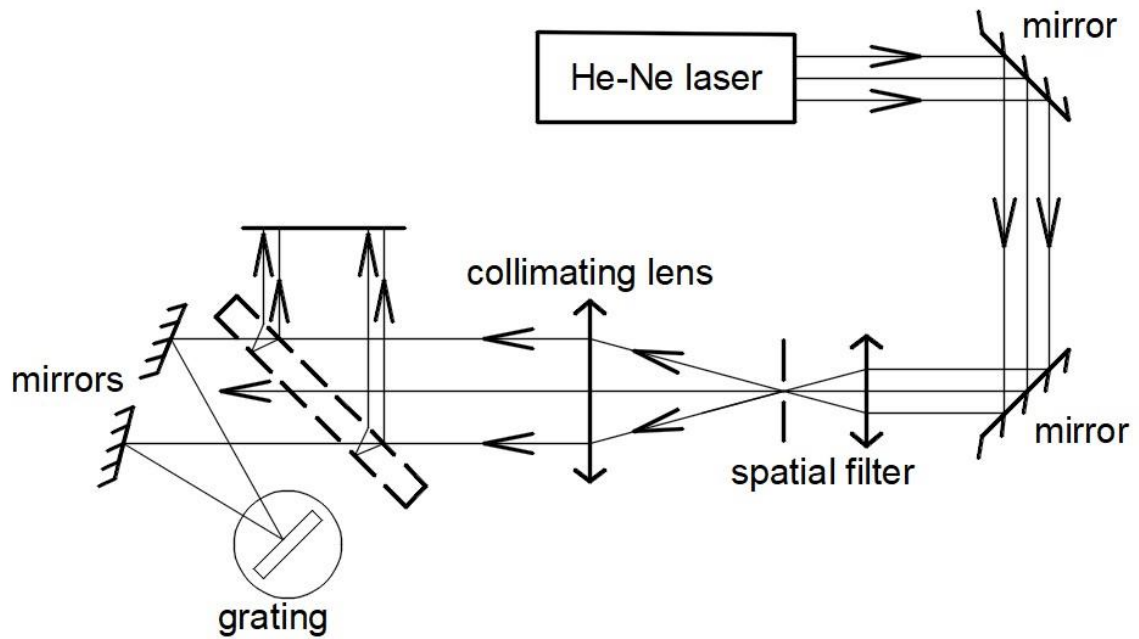


Figure 20 – making of the diffraction grating

The setup looked like this:

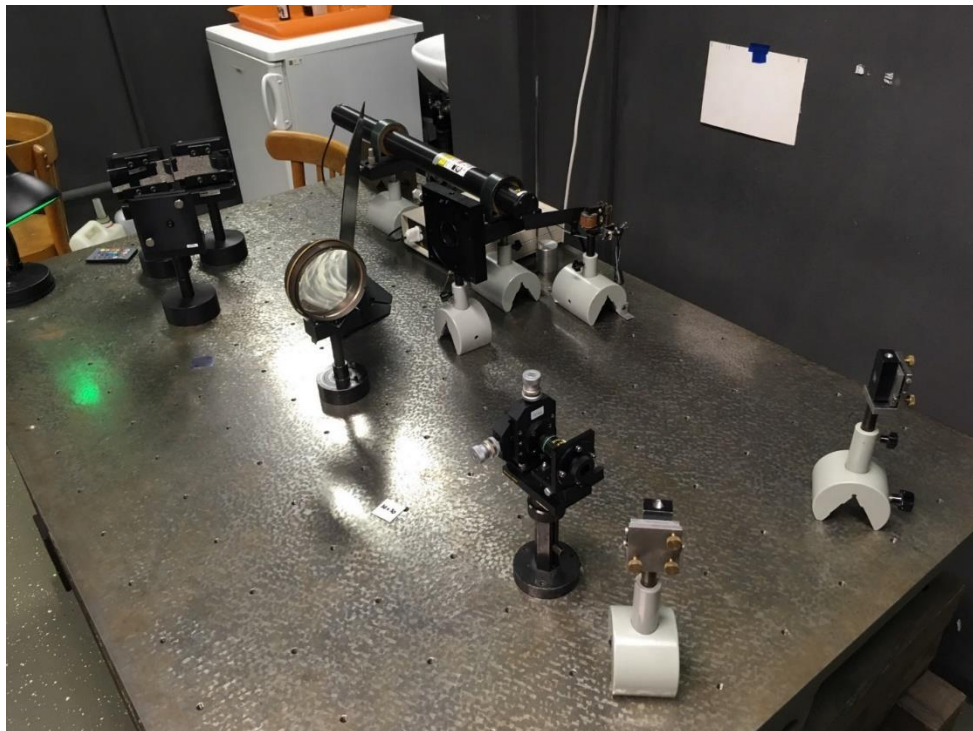


Figure 21 – making of the diffraction grating

The light from Helium-neon laser (wavelength of 632.8 nm) was expanded, split into two and was directed onto the small piece of holographic plate, where interference fringes of certain density are formed. The reason for that is interference. Depending of the angle between the two beams, different density can be reached, as there would be different distance between constructive intersections.

$$e = \frac{\lambda}{2 \cdot \sin \alpha} \quad [21]$$

Where e is a groove width and α is an angle between two beams.

The procedure was the following: first, the set up was prepared; then, the lights were off and the piece was put to the holder; after that, the laser was turned on for 0.2 seconds; after the exposure, the plate was put in a solution of CW-C2 developer, washed, bleached in a solution, contents of which could be found in the attachment #5, and finally washed and dried.

As it was difficult to reach the desired angle of interference, actual density differed from the desired, so it appeared to be 311.1451 grooves per 1 mm. The table of angles and density can be found in the attachment #6.

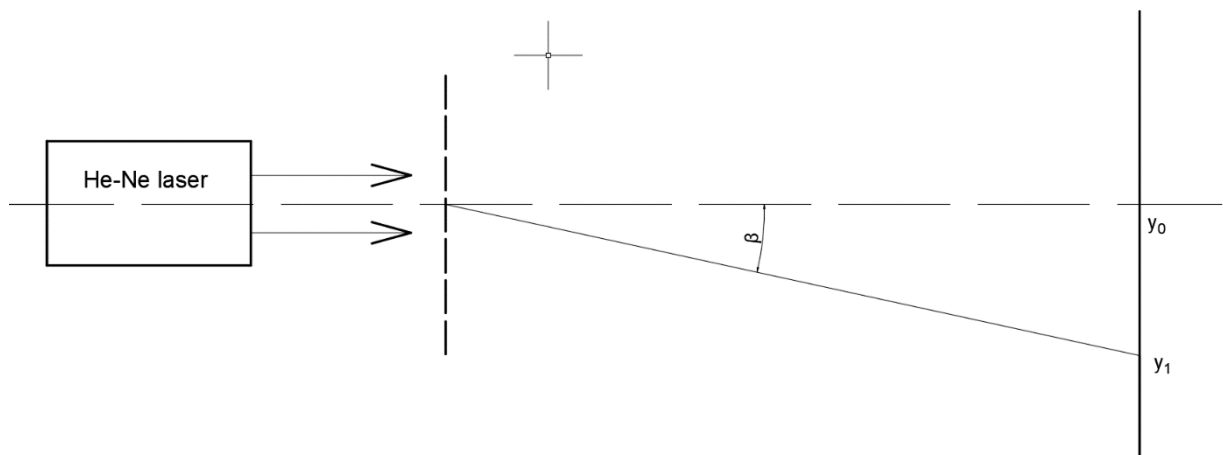


Figure 22 – measuring the grating density

The experiment of measuring the actual grating density was conducted as following. The light of known wavelength (He-Ne laser, λ is 632.8 nm) is passed through the grating that was made, the diffracted light was seen at the screen. Knowing the relation between wavelength, angle of diffraction and grating density, the last value can be calculated. Angle of diffraction was

calculated as an arctg of the relation of two distances. First is the distance from the grating to the screen, second is the distance from the normal to the first order of diffraction.

Knowing the actual diffraction grating, it is now possible to calculate the actual resolving power by using the formula from the equation 19. Using the same Matlab program as in the attachment #4, the actual resolving power of 1.887 nm is obtained.

Combining the equations 14 and 15 it is possible to get the formula for linear dispersion:

$$\frac{\partial l}{\partial \lambda} = \frac{d \cdot \cos \beta}{j \cdot f_{cam}} \quad [22]$$

The picture of the complete device without the upper part is shown below:



Figure 23 – complete assembly of the device

Calibration

After the device was finished, it was possible to perform the calibration. The constructed spectrometer was used to get the spectre of a mercury lamp. The setup of the experiment was simple: it was a room without any light but the mercury lamp. The phone with the spectrometer attached was pointed to the lamp. The results might have been affected by the automatic focusing, which was not possible to get deactivated. Therefore, the picture received was not as clear as it would be without automatic focusing.

The final spectrum of the mercury lamp received by using the constructed spectrometer is compared with the given spectrum and is presented below:

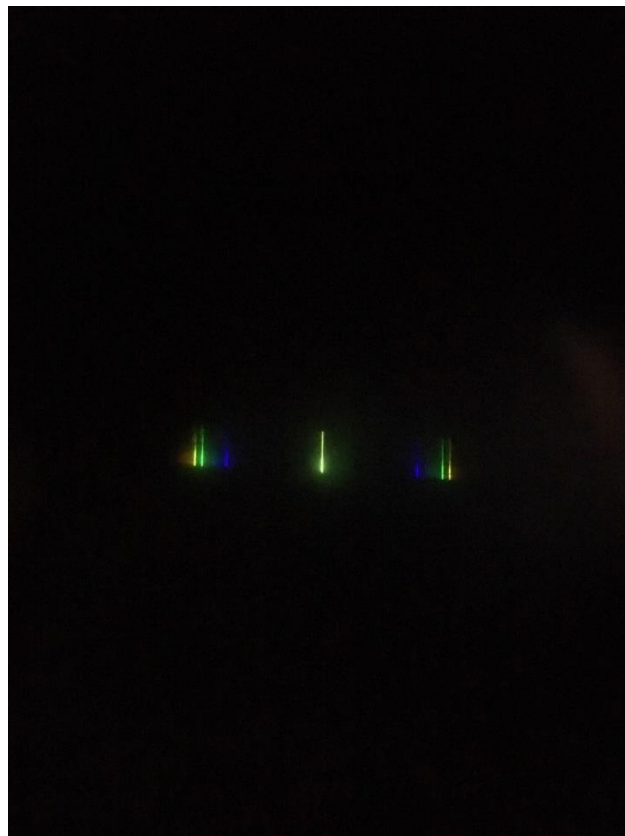


Figure 24 – mercury lamp spectrum

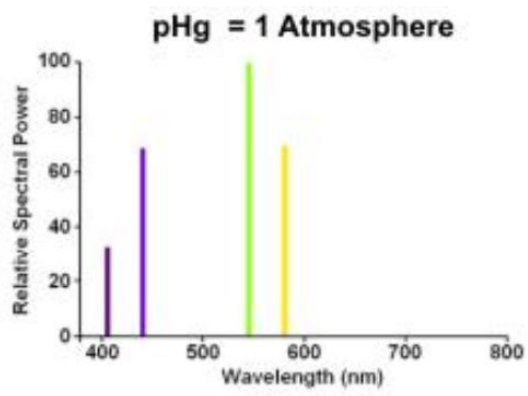


Figure 25 – given mercury spectrum [41]



Figure 26 – HG-2 spectrum [44]

Conclusion

The picture received from the spectrometer shows -1st, 0th and 1st orders of diffraction. It is seen clearly, on the figure 24, that there are three strips of different colors: yellow, green and blue for both 1st and -1st orders.

From the figures 25 and 26 it is possible to see that the 3 lines that are visible on the picture received from the spectrometer are of the following wavelengths:

- 435.833 nm (blue)
- 546.074 nm (green)
- 576.960 nm (yellow)

The goal of calibration is to find the error of the spectrometer by comparing two values: first is the distance from normal (0th order) to the lines of spectrum of known frequency that are calculated by using the grating equation:

$$\sin\beta = \frac{\lambda * m}{d} \quad [23]$$

Knowing the angle and the focal length of the camera, it is possible to calculate the distance using trigonometry:

$$y_n = \tan\beta * f'_{cam}$$

After that, we can compare this value to the one received from the spectrometer. Software IrfanView was used to count the pixels from 0th order to the spectrum lines, then this number was multiplied by the size of the pixel – 2.44 μm . The results of the calculations are shown in the table below.

Wavelength [nm]	Angle of diffraction [°]	Calculated distance [mm]	Pixels [-]	Measured distance [mm]	Error [%]
435.833	7.82	0.579	235	0.573	1.04
546.074	9.65	0.717	296	0.722	0.69
576.960	10.15	0.755	314	0.766	1.45

Table 3 – the results of the experiment

As the table shows, the results are quite close to the calculated values. Such a small error was not expected, as there were several sources of error. Some parts of the experiment could cause an error. The 3D printed model is not as precise as its computer model since the compound is expanded during the process of printing, therefore it could affect the distance between the entrance slit and the collimating lens. The focal length of the lens was also measured with some error. The grating density measurement error did also take place, as the distances were measured manually.

Despite the overall success of the work done, the spectrometer and the calibration part could be improved. Ideally, the experiment would have been done several times with different light sources. It would give more data to process; therefore, it would be more reliable. Also, the spectrometer itself could be created more precise. It would be reached by making the diffraction grating of higher grating density. That would proportionally increase the resolving power.

References

1. John Oliver Stoner, Jack D. Graybeal, George Samuel Hurst, Steven Chu. *Spectroscopy*. [Online]. Available from: <https://www.britannica.com/science/spectroscopy>
2. Dyna Whiting. *What is a spectrometer?* [Online]. Available from: <https://sciencing.com/spectrometer-5372347.html>
3. Dr. W. Kullmann and B. Keßler. *Optical Spectroscopy in Biomedical research*. [Online]. Available from: <https://andor.oxinst.com/learning/view/article/optical-spectroscopy-in-biomedical-research>
4. Harvard Medical School. *Blue light has a dark side*. [Online]. Available from: <https://www.health.harvard.edu/staying-healthy/blue-light-has-a-dark-side>
5. Michael and Lorna Herf. *Measuring the brightest iPhone ever*. [Online]. Available from: <https://justgetflux.com/news/2018/02/16/OLED.html>
6. Ulrike Holzgrabe, Iwona Wawer and Bernd Diehl. *NMR Spectroscopy in Pharmaceutical Analysis*. [Online] Available from: <https://www.sciencedirect.com/book/9780444531735/nmr-spectroscopy-in-pharmaceutical-analysis>
7. Rachel Metz. *A gadget for spotting fake Viagra, and other counterfeit pills*. [Online] Available from: <https://www.technologyreview.com/s/546076/a-gadget-for-spotting-fake-viagra-and-other-counterfeit-pills/>
8. <https://oceanoptics.com/spectroscopy-for-food-analysis/> [Online] Accessed on 15 May 2019.
9. Dieter Bingemann. *Near-Infrared Spectroscopy Probes Food Freshness*. [Online] Available from: <https://www.photonics.com/Articles/Near-Infrared Spectroscopy Probes Food Freshness/a61511>
10. Wikipedia. *Astronomical spectroscopy*. [Online] Available from: https://en.wikipedia.org/wiki/Astronomical_spectroscopy
11. Jim Lucas. *What is electromagnetic radiation?* [Online] Available from: <https://www.livescience.com/38169-electromagnetism.html>
12. Compound Interest. *The history of the atom – theories and models*. [Online]. Available from: <https://www.compoundchem.com/2016/10/13/atomicmodels/>
13. Encyclopaedia Britannica. *Bohr model*. [Online]. Available from: <https://www.britannica.com/science/Bohr-atomic-model>

14. R Nave. Quantized Energy States. [Online]. Available from: <http://hyperphysics.phy-astr.gsu.edu/hbase/Bohr.html>
15. <http://physics.tutorvista.com/waves/frequency-to-wavelength.html> [Online] Accessed on 22 May 2019.
16. Toppr. *Propagation of electromagnetic waves*. [Online]. Available from: <https://www.toppr.com/guides/physics/communication-systems/propagation-of-electromagnetic-waves/>
17. Encyclopaedia Britannica. *Electromagnetic spectrum*. [Online]. Available from: <https://www.britannica.com/science/electromagnetic-spectrum>
18. Mini Physics. *The electromagnetic spectrum*. [Online] Available from: https://www.miniphysics.com/electromagnetic-spectrum_25.html
19. Siyavula. *Electromagnetic spectrum*. [Online] Available from: <https://www.siyavula.com/read/science/grade-10/electromagnetic-radiation/11-electromagnetic-radiation-03>
20. Study.com. *Infrared radiation: Definition, Uses & Effects*. [Online] Available from: <https://study.com/academy/lesson/infrared-radiation-definition-uses-effects.html>
21. MedlinePlus. *X-Rays*. [Online] Available from: <https://medlineplus.gov/xrays.html>
22. Claire Gillespie. *What are the uses of ultraviolet light?* [Online] Available from: <https://sciencing.com/uses-ultraviolet-light-5016552.html>
23. <https://sciencing.com/uses-do-gamma-rays-8286669.html> [Online] Accessed on 25 May 2019
24. Encyclopaedia Britannica. *Planck's radiation law*. [Online] Available from: <https://www.britannica.com/science/Plancks-radiation-law>
25. Wikipedia. *Black-body radiation*. [Online] Available from: https://en.wikipedia.org/wiki/Black-body_radiation
26. Gigahertz-Optik. *Reflection, transmission and absorption*. [Online] Available from: <https://gigahertz-optik.de/en-us/basics-light-measurement/light-color/reflec-trans-abs/>
27. Nagibina I. M., Prokofiev V. K. (1967) *Spectral Instruments and Spectroscopy* (pp. 7-53)
28. Assignment point. *Dispersion of Light*. [Online] Available from: <https://www.assignmentpoint.com/science/physics/dispersion-light.html>
29. J. M. Derochette. *Index of refraction measurement*. [Online] Available from: http://jm-derochette.be/index_measurement/Theory.htm

30. Solverbook.com. *Diffraction spectrum*. [Online] Available from:
<http://ru.solverbook.com/spravochnik/fizika/difrakcionnyj-spektr/>
31. *Diffraction and interference*. [Online] Available from:
http://electron6.phys.utk.edu/phys250/modules/module%201/diffraction_and_interference.htm
32. Kris Walker. *Spectrometer Technology and Applications*. [Online] Available from:
<https://www.azom.com/article.aspx?ArticleID=10245>
33. Bwtek. *How does a spectrometer work?* [Online] Available from:
<http://bwtek.com/spectrometer-introduction/>
34. Wikipedia. *Spectroscopy*. [Online] Available from:
<https://en.wikipedia.org/wiki/Spectroscopy>
35. Encyclopaedia Britannica. *Spectrochemical analysis*. [Online] Available from:
<https://www.britannica.com/science/spectrochemical-analysis>
36. Jim Clark. *The fingerprint region of an infra-red spectrum*. [Online] Available from:
<https://www.chemguide.co.uk/analysis/ir/fingerprint.html>
37. Device specifications. *Device specifications of iPhone SE*. [Online] Available from:
<https://www.devicespecifications.com/ru/comparison/82736b95f>
38. OpenStax. *Mathematics of interference*. [Online] Available from:
[https://phys.libretexts.org/Bookshelves/University_Physics/Book%3A_University_Physics_\(OpenStax\)/Map%3A_University_Physics_III_-_Optics_and_Modern_Physics_\(OpenStax\)/03%3A_Interference/3.03%3A_Mathematics_of_Interference](https://phys.libretexts.org/Bookshelves/University_Physics/Book%3A_University_Physics_(OpenStax)/Map%3A_University_Physics_III_-_Optics_and_Modern_Physics_(OpenStax)/03%3A_Interference/3.03%3A_Mathematics_of_Interference)
39. OpenStax. *Young's Double Slit Experiment*. [Online] Available from:
<https://opentextbc.ca/physicstestbook2/chapter/youngs-double-slit-experiment/>
40. Ibsen. *Spectrometer design guide*. [Online] Available from:
<https://ibsen.com/technology/spectrometer-design-guide/>
41. Lamptech. *The effects of mercury vapour pressure*. [Online] Available from:
<http://lamptech.co.uk/Documents/M3%20Spectra.htm>
42. R Nave. *Thin-Lens equation:Newtonian form*. [Online] Available from:
<http://hyperphysics.phy-astr.gsu.edu/hbase/geoopt/lenseq.html>
- 43 [Online] Available from: <https://www.deviceranks.com/ru/camera-sensor/107/sony-imx315-exmor-rs>

44 [Online] Available from: <https://shop.spectrecology.com/product/wavelength-calibration-sources-hg-2-ar-2-kr-2-ne-2-xe-2/>