



Setup of a Fourier Transform Infrared Spectrometer

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1 Introduction

Most of our knowledge about the structure of atoms and molecules is based on spectroscopic investigations. Atoms within a molecule are constrained by molecular bonds to move together in a certain specific ways, called degrees of freedom. These are: electronic, translational, rotational and vibrational. In electronic motion, the electrons change energy levels or directions of spins. The translational motion is characterized by a shift of an entire molecule to a new position. The rotational motion is described as a rotation of the molecule around its center of mass. When the individual atoms within a molecule change their relative position, we say that the molecule vibrates. The vibrational transitions are the most important transitions for IR spectroscopy because infrared spectra result from transitions between quantized vibrational energy states [1].

A major breakthrough in IR spectroscopy was the introduction of Fourier transform infrared (FTIR) spectrometers which used interferometers. FTIR spectroscopy is one of the techniques that are used today for measuring the intensity of infrared radiation as a function of frequency or wavelength. In the 1820s Lord Rayleigh recognized that the output from an interferometer could easily be converted to a spectrum using a mathematical operation Fourier transformation.

An essential part of the hardware of a FTIR spectrometer is the IR source. The properties of laser radiation (monochromaticity, coherence, directionality, brightness) and the possibility that lasers can operate in continuous or pulsed mode, make these devices preferable tools for spectroscopy. A laser can also be used to control the velocity of the moving mirror, to time the collection of data points throughout the mirror stroke and as a reference signal within the instrument.

The goal of this report is to set up a FTIR interferometer with computational control and to measure the spectra from different light sources : CW alignment laser and a femtosecond pulsed laser. A comparison between the FTIR spectroscopy and the autocorrelation technique is discussed.

2 Theory

2.1 What is Fourier transform spectroscopy how does it work?

Fourier transform infrared spectroscopy studies the interaction of infrared light with matter. Analysis of infrared spectrum can give both quantitative and qualitative analysis- i.e. it can tell you what type of molecules are present in a sample and at what concentrations. This technique can obtain spectra from wide number of samples in gas, liquid or solid state and study their structure.

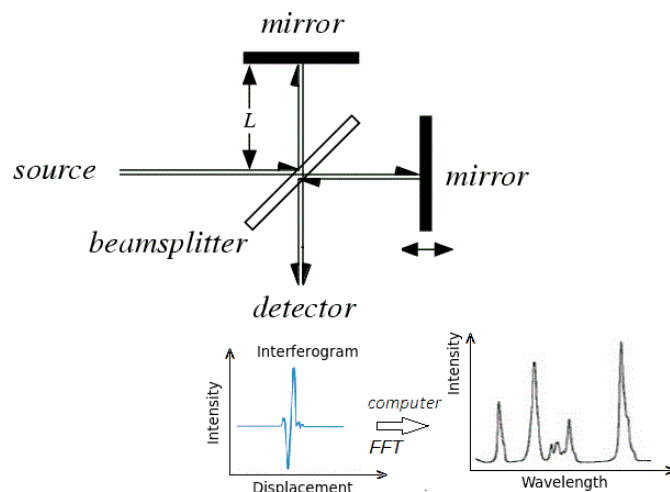


Figure 1: Sketch of a FT-IR spectrometer. Partially taken from [2].

In figure 1 is presented schematic representation of most widely used set-up for FTIR spectrometer. Light from an infrared source is split into two arms of Michelson interferometer by a beam-splitter, a device that ideally, allows 50% of light to pass through to the movable mirror while reflecting the other 50% to the fixed mirror. The beam that travels to the fixed mirror is reflected and returns to the beam splitter again, after a total optical path length of $2L$. The same happens to the beam that is transmitted by the beam splitter in the direction of the movable mirror. Once the light beams reflect from these mirrors they travel back to the beam-splitter, where they are recombined into a single light beam, and because of their spatial coherence they interfere constructively or destructively. The result from the interference is dependent on their optical path difference δ [3]. The light beam reflected from the fixed mirror and the light beam reflected from the moving mirror travel the same distance at the same speed. Thus when the two beams recombine at the beam-splitter they are in phase with each other, and they constructively interfere, giving a final beam more intense than either of the two beams by themselves. Then the optical path difference is multiple of their wavelength:

$$\delta = m\lambda,$$

where δ is the Optical path difference,
 λ is the Wavelength of the infrared source,
 $m = 0, 1, 2, \dots$, any integer.

On the other hand destructive interference occurs when the two beams are some number of cycles plus a half out of phase with each other. Thus, we can write for destructive interference that:

$$\delta = \left(m + \frac{1}{2}\right) \lambda.$$

Another thing that need to be discussed is the distance the mirror moves. The mirror displacement is denoted as Δ . A mirror translation of Δ gives an optical path difference of 2Δ because the light traverses the displaced distance twice on the way to and from the moving mirror. This is shown in figure 2.

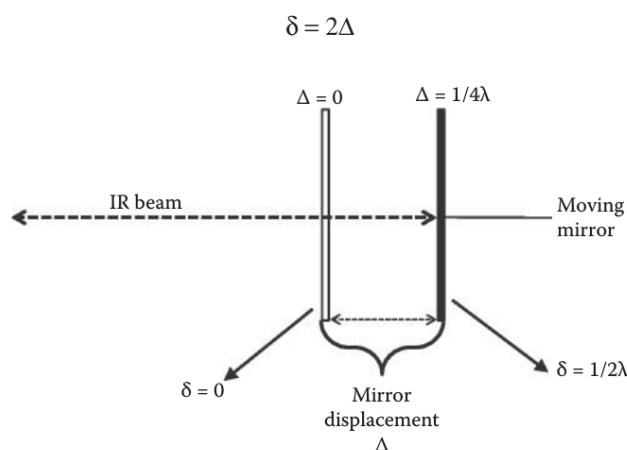


Figure 2: An illustration of how moving the mirror in a Michelson interferometer produces a non-zero optical path difference. The optical path difference is twice mirror displacement because the light beam traverses the extra distance twice. [3]

After the recombination, the whole beam is then again partially transmitted and partially reflected by the beam splitter. The reflected beam is then focused on the detector. The intensity directly recorded by the detector is a function of the displacement of the moving mirror and it is called a raw data or an interferogram. What we need in fact is the intensity as a function of the wavelength or frequency- i.e. the spectrum, which can be easily obtained in a computer using a simple fast Fourier transform code. This is explained in section 2.2.

2.1.1 Characteristics of FTIR

In this section some important parameters of FTIR Spectroscopy are going to be explained [3],[4].

- Resolution:

The resolution of a spectrometer is a measure of how well an instrument distinguishes peaks that are close together. Since interferogram data points are obtained at evenly spaced intervals, high-resolution scans require more data points and hence greater optical path differences than low-resolution scans. Thus there is a relationship between resolution and optical path difference as follows:

$$\text{Resolution} \propto 1/\delta.$$

-Signal to noise ratio: One of the most challenging problems in interferometry and in many other fields in physics is to extract an useful signal from the noisy background. The characteristic term is the signal-to-noise ratio (SNR). In spectroscopy there is a relation between SNR and the resolution of the scan:

$$\text{Resolution} \propto \text{SNR}.$$

So high-resolution spectra contains more information, but are inherently noisy.

- Number of scans: The goal of modern physics is to get faster and easier measurements, without reducing its quality. So another parameter that should be take into account is the number of scans N . Analysis time t is proportional to the number of scans, so more scans, more time will take. There is another relation that shows that the resolution is proportional to square root of the number of scans:

$$\text{Resolution} \propto N^{1/2} \propto t^{-1}.$$

At the end we have to note that high-resolution scans are noisier and longer than the low-resolution scans. So there is no universal recipe for FTIR spectroscopy and all the parameters are dependent on the sample that is used and the concrete experiment conditions.

2.1.2 Advantages and disadvantages of FTIR

In this section are going to be presented the advantages and disadvantages of FTIR Spectroscopy [5], [6].

a1. The main advantage of Fourier spectroscopy is the fact, that all spectral intervals are measured simultaneously (at the same time), in contrast to classical spectroscopy with a monochromator, where the different spectral intervals are measured subsequently [5]. The interferometer does not separate energy into individual frequencies for the measurement. Each point in the interferogram contains information from each wavelength of light being measured. Every stroke of the moving mirror equals one scan of the entire infrared spectrum, and individual scans can be combined to allow signal averaging. This is called the Multiplex or Fellgett's advantage.

a2. Many types of samples including solids, liquids, gases, semi-solids, powders, polymers, organic, inorganic, biological materials, pure substances, and mixtures have strong

Table 1: Advantages and Disadvantages of Fourier Transform Infrared Spectroscopy

Advantages	Disadvantages
a1.Fast and Easy	d1. Cannot detect some molecules
a2.Almost Universal	d2. Mixtures
a3.Spectrum is information rich	d3. Water
a4.High Sensitivity and SNR	
a5.Non destructive	
a6.Mechanically simple	

absorbency in the mid-infrared, hence one achieves good specificity.

a3. The peak positions give the structures of the molecules in a sample, the peak intensities give the concentrations of molecules in a sample, and the peak widths are sensitive to the chemical matrix of the sample.

a4. The FTIR instrument does not limit the amount of light reaching the detector - more radiation can be passed between the source and the detector for each resolution element. Higher signal leads to higher SNR and this means greater resolution The energy throughput is higher for any resolution,giving a higher SNR. This is called the throughput or Jacquinot's advantage.

a5. The IR light does not damage the used samples.

a6. The FTIR Spectrometer contains only one moving part.

d1. Individual atoms (such as the noble gases helium and argon), mono-atomic ions, a single atom with a charge,and homo-nuclear diatomic molecules (such as O₂ or N₂) do not have an infrared spectrum.

d2. The more complex the composition of a sample, the more complex its spectrum becomes, and the more difficult it is to determine what peaks are from what molecules.

d3. Liquid water is a problem because its broad and intense peaks can mask the spectra of solutes dissolved in water.

2.2 Fourier transformation

As mentioned before earlier Fourier transformation is required to convert the raw data into the actual spectrum. A simple explanation of what a Fourier transform is the following: it transforms any time dependent function to a function in frequency domain.

The intensity from the IR source, recorded by the detector (see for example figure 1.) can be presented as [7]:

$$I(\Delta) = \frac{1}{2} \int_0^\infty I(\sigma)(1 + \cos(2\pi\sigma\Delta))d\sigma.$$

This signal is composed by unmodulated and modulated parts:

$$I_u = I(\Delta) = \frac{1}{2} \int_0^\infty I(\sigma)d\sigma.$$

$$I_m = I(\Delta) = \frac{1}{2} \int_0^\infty I(\sigma) \cos(2\pi\sigma\Delta)d\sigma.$$

The modulated part is called the interferogram. If we let that the spectral signal is symmetrical about some central σ_0 and then the distribution can be shifted by $-\sigma_0$ to make the distribution as an even function, then the interferogram can be expressed as:

$$I(\Delta) = \frac{1}{2} \int_{-\infty}^\infty I(\sigma)(\cos(2\pi\sigma\Delta) + \iota \sin(2\pi\sigma\Delta))d\sigma = \frac{1}{2} \int_{-\infty}^\infty I(\sigma)e^{2\pi\sigma\Delta}d\sigma.$$

Since the intensity as a function of wavenumber $I(\sigma)$ is real even function, the imaginary odd part will vanish after integration. Then the intensity as a function of displacement of the moving mirror $I(\Delta)$ is still a real function. Finally we see that the intensity as a function displacement and the intensity as a function of wavenumber for a Fourier Transform pair, so it can be recovered from the interferogram by Fourier transformation:

$$I(\sigma) = 2 \int_{-\infty}^\infty I(\Delta)e^{-2\pi\sigma\Delta}d\Delta.$$

In practice the movable mirror moves with constant velocity and the detector will record the total intensity as a function of time, which is actually a function of mirror displacement, considering the constant velocity.

2.3 Comparison of linear and nonlinear autocorrelation

FTIR spectroscopy is a good technique for receiving the spectra from different types of light sources working in both CW and pulse regime.

Ultrashort laser pulses have become a ubiquitous tool in natural sciences and their characterization is of fundamental importance. Because of the short time interval in the femtosecond region, we cannot use standard apparatus for visualization and analyzing these light pulses. Indirect correlation measurement techniques have to be applied, making use of interferometry and nonlinear processes.

The autocorrelation is a technique based of comparison between a given signal and its identical copy at different points in time. The similarity of two functions is measured by a correlation integral and the function which is received after its solving is called correlation function. If these two functions are the same this is called autocorrelation. This can give us a method for estimation the duration of the pulse in time domain. That is what exactly distinguishes the FTIR spectroscopy from autocorrelation.

The setup from figure 1 can be easily converted to autocorrelation scheme if before the detector, we put a lens and a nonlinear crystal. For profound introduction with the autocorrelation technique see references [8] and [9].

3 Experimental setup and results

The main goal of the project was to build a Fourier transform interferometer that collects spectra in the infrared spectral region and which is controlled by a computer. Spectra from two light sources are analysed:

- CW alignment laser in the visible spectral region.

- Yb:KGW femtosecond laser system in the infrared spectral region

The first one serves as a calibration source of the system. And the second one is a real IR laser source.

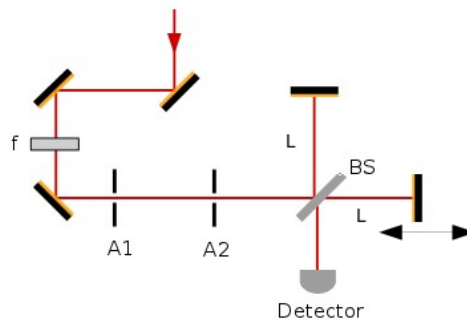


Figure 3: Experimental Setup. f = filter for the green component of the laser radiation, $A1, A2$ = apertures, BS = beam splitter

Figure 3 shows the experimental setup. This is how the setup looks like with the use of femtosecond laser. Since for the CW alignment laser no filtration is needed, the source is at the place of the third mirror.

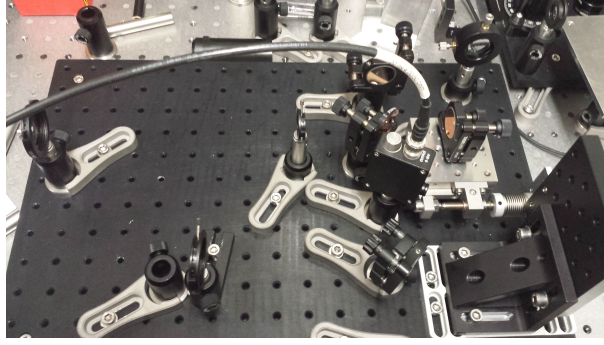


Figure 4: Real picture of the experimental setup.

The input beam passes two mirrors, is then transmitted through a filter that damps the green (515 nm) component of the radiation of the femtosecond laser. Then the beam passes two apertures, and enters the Michelson interferometer. We use metallic gold mirrors, pellicle beam splitter with R/T Ratio of roughly 45% to 55%. An Si photo detector is used for the CW alignment laser, and faster InGaAs photo detector for the fs laser system.

3.1 CW alignment laser

A laser pointer with central output wavelength of about $\lambda = 650 \text{ nm}$ and an output power $P = 10 \text{ } \mu\text{W}$ is used.

Scan for 8000 steps with speed 5 steps per second (or 0.8 microns per second) to receive the interferogram. Resolution of $0.03 \text{ } \mu\text{m}^{-1}$ is achieved.

In figure 5. is presented the interferogram and the spectrum of the alignment laser.

Figure 6 shows how the spectrum of the alignment laser looks like and serves for a comparison. As seen from that the expected peak is observed, but it is wide and the spectrum is a lot noisy.

3.2 Femtosecond Yb:KGW laser

Commercial laser system from LIGHT CONVERSION is used, which consists of a Yb:KGW laser oscillator with a regenerative amplifier and an optical parametric amplifier. The fundamental the laser oscillator has an output wavelength of about 1030 nm, a repetition rate of 5 kHz, a pulse duration down to 150 fs and a maximum pulse energy of up to 1 mJ. The optical parametric amplifier enables a broad range of wavelength conversion ranging from 600 to 2720 nm, whereas the used idler beam can be tuned from 900-2720 nm. [10].

First a idler wavelength of $\lambda = 1500 \text{ nm}$ is chosen. I scan to find the position where the two beams overlap completely. Then i scan for 240 micrometers, which equals of 8000

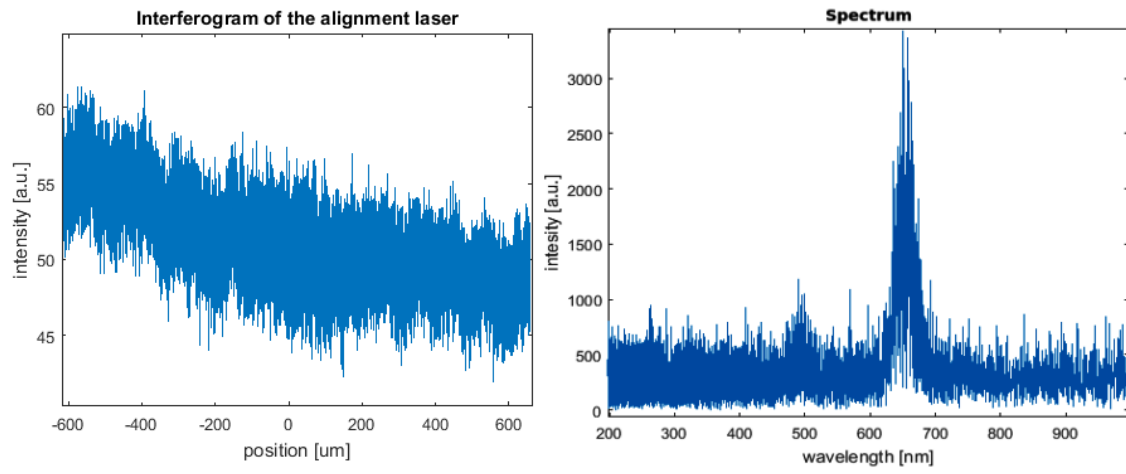


Figure 5: Interferogram (left) and Spectrum in wavelength (right) of CW Alignment laser.

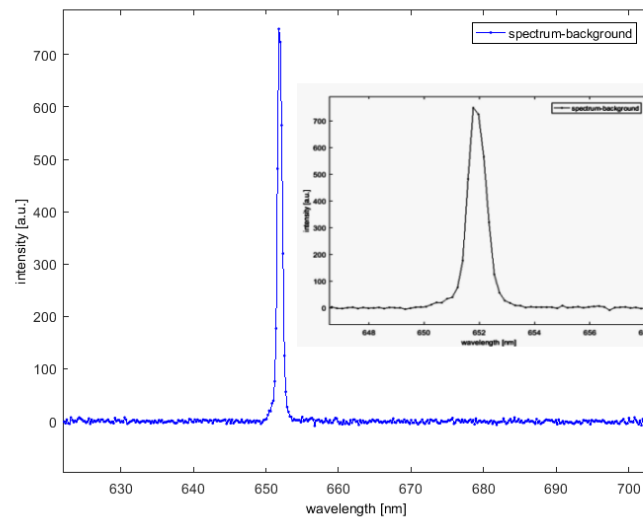


Figure 6: Reference spectrum of the CW Alignment laser

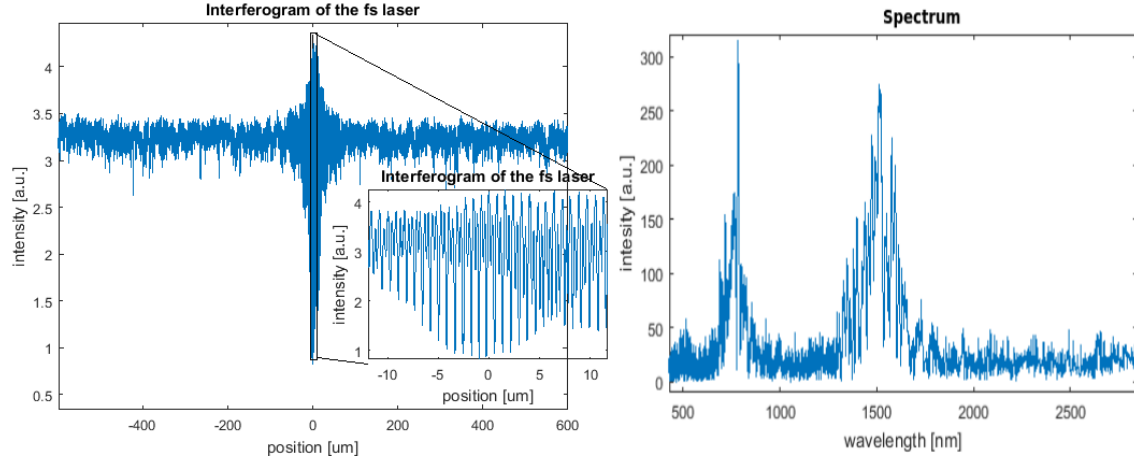


Figure 7: Interferogram (left) and Spectrum in wavelength (right) of fs Yb:KGW laser.

steps of the stepper motor with speed 10 steps per second to receive the interferogram.

In figure 7 are presented both the interferogram and the spectrum of the fs laser.

Since we use a Optical parametric amplifier, we can see the three output wavelengths - the idler $\lambda = 1500 \text{ nm}$, the pump $\lambda \sim 515 \text{ nm}$, and the signal wave $\lambda \sim 800 \text{ nm}$.

4 Summary

The Fourier Transform Infrared Spectrometer is the most widely used type of infrared spectrometer, which is used to obtain spectra from different sources and samples. The benefits of using a FTIR spectrometer are excellent spectral quality, high data collection speed, good reproducibility of data, and ease of maintenance and use. In this work a FTIR Spectrometer is build, with the purpose to collect spectra from light sources in Infrared spectral region. Using a motorized delay stage controlled by a custom written LabVIEW program, temporal overlap of the two beams is established. Then an interferogram is collect scanning for 8000 steps with speed 10 steps per second around the interference pattern or said another way 58 position per second can be measured. For the alignment laser a resolution of $0.03 \text{ } \mu\text{m}^{-1}$ is achieved. The resolution can be improved by increasing the SNR or the scanning time. The scans took 45 minutes in total (15 minutes for the fs laser and 30 minutes for the alignment laser). The spectrograms are analysed on a computer using Fourier transformation code written in Matlab.

The results are as they were expected. From spectra we can estimate that the output wavelength for the calibration laser is $\lambda = 650 \text{ nm}$ and for the IR laser source - idler wave $\lambda = 1500 \text{ nm}$, pump wave $\lambda \sim 515 \text{ nm}$, and the signal wave $\lambda \sim 800 \text{ nm}$. As a future development this setup can be easily converted in nonlinear autocorrelation scheme when a lens and a nonlinear crystal are put before the detector. It can then give information about the pulse duration.

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