Development of an Economical, Linear CCD Based Spectrometer

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Abstract

Spectrometry provides vital information about the composition of electromagnetic radiation by measuring wavelengths of light over a wide range of the electromagnetic spectrum. In this work, design and construction of an economical linear CCD spectrometer and a computer application is presented. A sample of the light source travelling through an optical fiber enters the device and the spectrum produced by a diffraction grating is projected on a linear CCD detector. The data is sampled using a 10-bit ADC to the microcontroller memory and finally transferred to the computer via a full speed USB connection. In the computer, the data is digitally processed and displayed through a graphical user interface with several useful functionalities. The device is sensitive to electromagnetic waves of wavelengths ranging from 400 to 800 nm, which is decided by the sensitivity of the silicon CCD detector. The device performs in par with commercially available handheld spectrometers and is equipped with wavelength and amplitude calibration capabilities.

Keywords: spectrometer, instrumentation, CCD

1. Introduction

Optical spectrometry is a widely used technique that enables the characterisation of materials based on their light absorption or emission profiles across ultra-violet (UV) to near-Infrared (NIR) region. This can provide valuable information about the chemical composition of materials in all states of matter and makes the technique ideal for the analysis of light sources such as lasers and light emitting diodes (LED) (Gornushkin, et al., 2000). In addition, optical spectrometers facilitate other advanced techniques including fluorescence (Morris, et al., 1994), irradiance (Kouremeti, et al., 2008), oxygen sensing (Chu, et al., 2007), pH sensing (Netto, et al., 1995), reflectance and transmittance of materials (Joyce et al, 2002) and Raman spectroscopy (Long, et al., 1977).

The basic structure of an optical spectrometer consists of a collimator, monochromator and a detector. Early advances in monochromator technologies resulted in ruled diffraction gratings which have high fidelity and are now universally used in digital spectrometers. A major leap in detector technologies came with the advent of the charge coupled device (CCD) (Fossum, et al., 2014). The CCD can capture the complete spectral window within the span of a few seconds allowing real-time dynamic measurements. As CCDs can be easily interfaced to a computer, data can be stored for post-processing indefinitely. Nowadays, top of the range spectrometers use thermo-electrically cooled, back-thinned, deep depleted CCDs along with high speed microcontrollers which are used to drive the CCD's to capture spectral data. These are then displayed using specialised proprietary software that enable spectral analysis (Williamson, et al., 1989) features in most commercial spectrometers are under-utilised in undergraduate laboratories. This makes digital spectrometers a rare educational tool, despite the many benefits that it can offer.

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Even in a research laboratory the lack of customisable open source application software coupled with the high-cost would not provide value for money especially in the context of a developing nation. Nevertheless, the global mass production of electronic components has brought down the price of devices and undergraduate laboratories could utilise this opportunity to fabricate their own requirements.

Here, the design and construction of an economical linear CCD based digital spectrometer device with complementary open source application software is presented. The instrument can be easily reproduced by novice students, and can be customised for basic teaching purposes or research by selecting components with suitable specifications.

2. Methodology

The design and construction of the spectrometer was done in stages which included the optical setup, CCD driver, computer application, calibration and an optional thermoelectric cooling module.

2.1 Optical setup

The primary function of the optical setup was to separate the incoming photons of different frequencies by means of diffraction. The light from the source or sample first arrives at a vertical slit, which acts as the entrance to the spectrometer. The beam then diverges on to a concave mirror which collimates and directs the light to the diffraction grating. The diffracted light is then sampled by the CCD placed at an optimum distance. In order to reduce optical losses in the vertical direction, a cylindrical lens is placed prior to the CCD as shown in Figure 1. The vertical slit had a width of 100 µm and was made of two razor blades. The light beam convergence was achieved by the use of a high reflective concave mirror from THORLABS. The selected concave mirror was an achromat with a dielectric coating optimised over 400-700 nm wavelength range with greater than 99% average reflectivity within this range. A concave mirror was preferred over a conventional convex lens to focus the light since the losses from a lens due to absorption by the lens material is typically much higher than in a mirror. The selected diffraction grating from THORLABS had a blaze wavelength of 500 nm, with a grating efficiency of about 55 % at 635 nm.

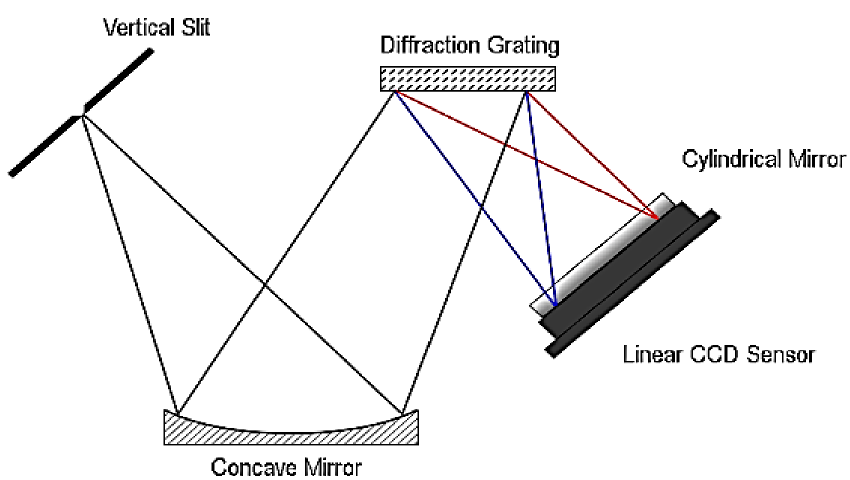

Figure 1. Component arrangement of the optical setup of the spectrometer.

2.2 CCD and driver circuit

The light dispersed from the grating was then captured by the CCD. Once calibrated against a known light source such as a Mercury lamp, each pixel in the array can be assigned a specific wavelength, which can facilitate the measurement of spectra. However, the *y* axis representing the intensity of the incident light is not generally calibrated as its' characteristics depend on each image sensor that is used. The CCD that was used for this work was the Toshiba TCD 1201 D. This particular CCD has 2,048 elements and a high sensitivity to low lights. The pixel size is 14×200 μm and has a dynamic range of 400 with a quantum efficiency of 95%.

The CCD was driven by an ATmega 328p microcontroller in an Arduino UNO development board. The microcontroller was used to generate the desired clock pulses for each control pin of the CCD as described in its datasheet. The in-built analogue-to-digital converter (ADC) was used for measuring the voltage of each individual pixel of the CCD. The data was transferred to the personal computer (PC) running the custom made application software via USB serial communication.

2.3 Computer application

Typically, the measured spectrum is initially displayed as a plot of ADC value versus the pixel number. After the calibration, the pixel number is replaced by the corresponding wavelength or frequency. The purpose of the computer application was to provide control signals to the microcontroller and gather, analyse and report spectrum data of the sample. Another important task governed by the application is the calibration of the device. The application stores calibration data in the local memory after a successful calibration session. To control and view the output spectrum and to perform the calibration of the device, windows based graphical user interface (GUI) was created using Microsoft visual studio 2017 using visual C# as the programming language.

2.4 Calibration

Calibration of the spectrometer consists of two steps involving wavelength calibration and amplitude calibration. Wavelength calibration was achieved with the use of a mercury lamp and semiconductor lasers as the light sources. The amplitude calibration was not carried out for this instrument as almost all applications require only a relative intensity value and therefore even commercial spectrometers do not offer an amplitude correction. However, based on the wavelength response data given by the CCD data sheet, an amplitude correction was performed to adjust for the wavelength dependent variation. The Table 1 shows the color, peak wavelength and the intensity of each wavelength in arbitrary units of a mercury lamp which was used to perform the wavelength calibration.

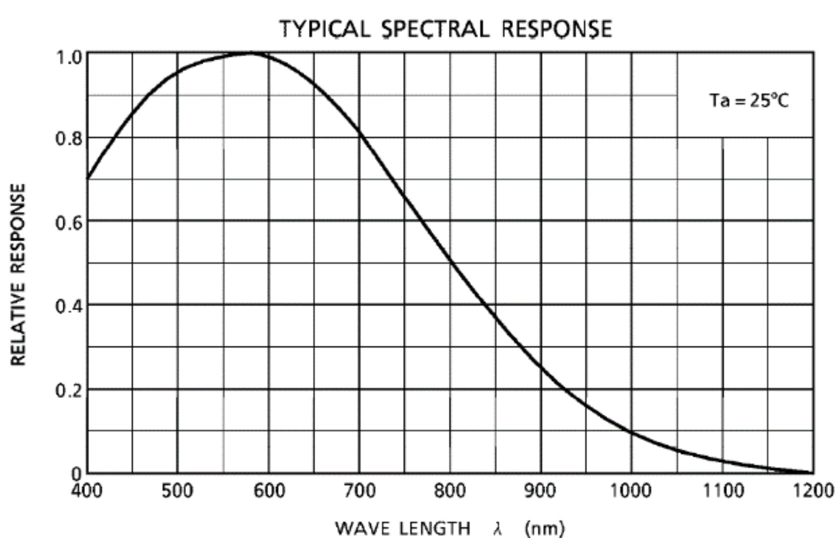

Figure **Error! No text of specified style in document.**. Wavelength response of TCD1201D linear CCD.

Table 1: Wavelength calibration peaks for the mercury lamp and the amplitude correction based on the wavelength response of the CCD.

Color	Wavelength (nm)	Amplitude (arb. units)
IR	1,128.700	-
IR	1,014.000	-
Yellow	579.054	1,000
Yellow	576.959	200
Green	546.074	2,000
Blue-green	491.604	50
Blue	435.835	500
Violet	407.781	150
Violet	404.656	300
UV	366.328	400
UV	365.483	200
UV	365.015	500

2.5 Thermoelectric cooling of the CCD

Thermoelectric cooler (TEC) is a solid state heat pump used in applications where temperature stabilisation and cycling or cooling is required. It consist of an array of p-n junctions, which when a direct current is passed through, can result in a net heat transfer from one surface to the other.

The temperature sensor module had perfect thermal contact with the cold junction of the thermoelectric cooler using an aluminum plate. This helped detect the required temperature level of the cooling side of thermoelectric cooler. The hot junction of the thermoelectric cooler was connected with a heat sink and a fan. The experimental system configuration is depicted in Figure 3. A 12V/9A power supply was used to supply the input power for the TEC. The temperature of the TEC mounting plate (Aluminum plate) was measured using the temperature sensor with an accuracy of .$\pm 0.5^{o}$ C.

An Arduino code was implemented to control the correct temperature of the TEC. Therefore, microcontroller based PID (Proportional–Integral–Derivative) (Bista et al., 2016) controllable cooling system was developed for cooling the CCD. The working mechanism of the temperature controller system can be summarised as below;

- The Arduino read the temperature of the sample using the temperature sensor, which was connected to the Arduino through analog-pin 8 as shown in the Figure 3.
- The received temperature value of the sample was compared with the setpoint temperature and the necessary digital outputs were given through four digital output pulse-width modulation (PWM) signals (PWM pins-6). These PWM signals were sent to the motor driver.
- The received PWM signals controlled the amount and the direction of the current across the TEC via motor driver.

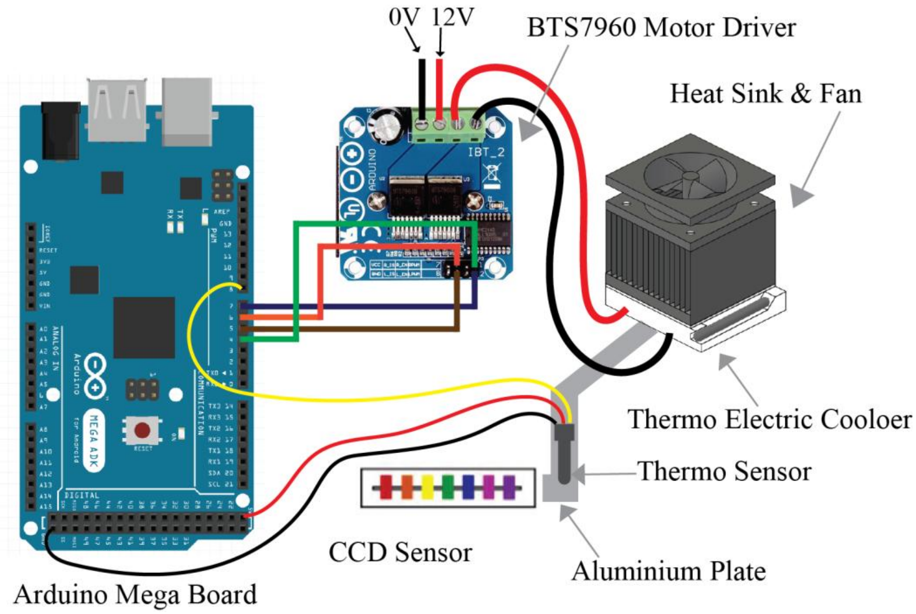

Figure 3. Circuit diagram and configuration of the cooling system.

3. Results and Discussion

In the final stage of the build, the optical and electronic components were enclosed in a custom-made enclosure made with 3 mm thick black acrylic boards (Figure 4). The opaque material prevented external light entering the spectrometer.

Figure 4. The custom-built spectrometer.

Figure 5 shows a screen capture of the computer application created for the spectrometer. The software supports both wavelength and amplitude calibration and additionally, dark signal and ambient signal compensation.

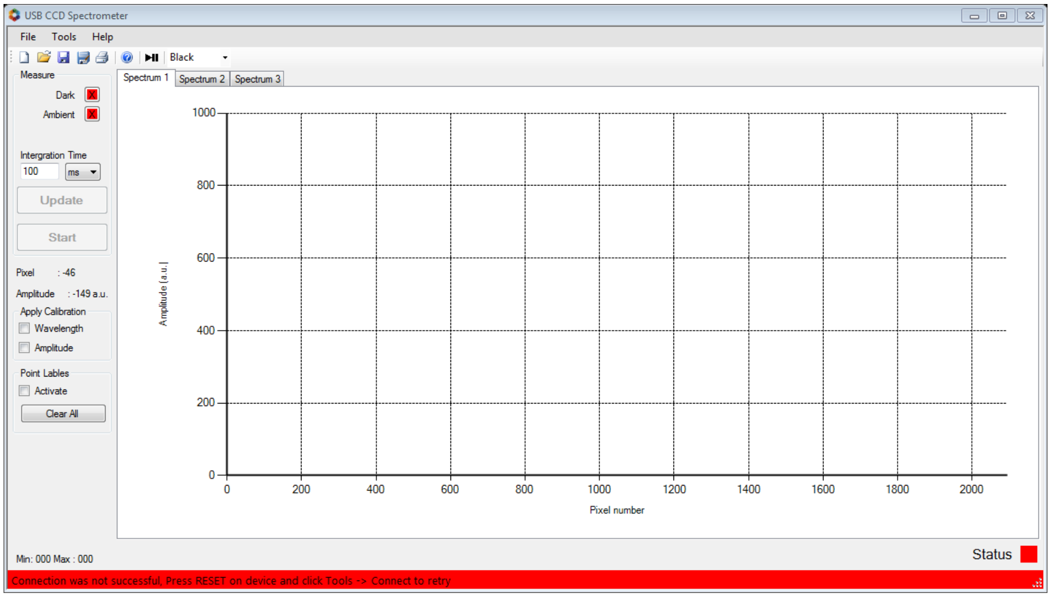

Figure 5. GUI of the computer application for the spectrometer.

The spectrometer was used in measuring emissions of several different light sources. Figure 6 and 7 show an emission spectrum of a precision laser diode module and household Compact Fluorescent Light (CFL) (nearly equal to pure mercury spectrum). Figure 6(b) is a spectrum of a CFL bulb that is acquired by a commercial spectrometer (Ocean Optics Flame). The comparison of the two spectra in Figure 6 reveals that the reported spectrometer has a raised middle portion of the spectrum than that of the commercial device, this is due to slight over-exposure of the CCD. Another indication for over exposure is the summit like appearance of major peaks, nevertheless this can be easily adjusted by reducing the exposure time and thus limiting the amount of light that is being sampled. A good exposure shows sharp Voigt profile peaks with minimum disturbance to the neighboring photocells. As seen from the results, the device performs well with very low noise profile depending on the intensity of the incident radiation.

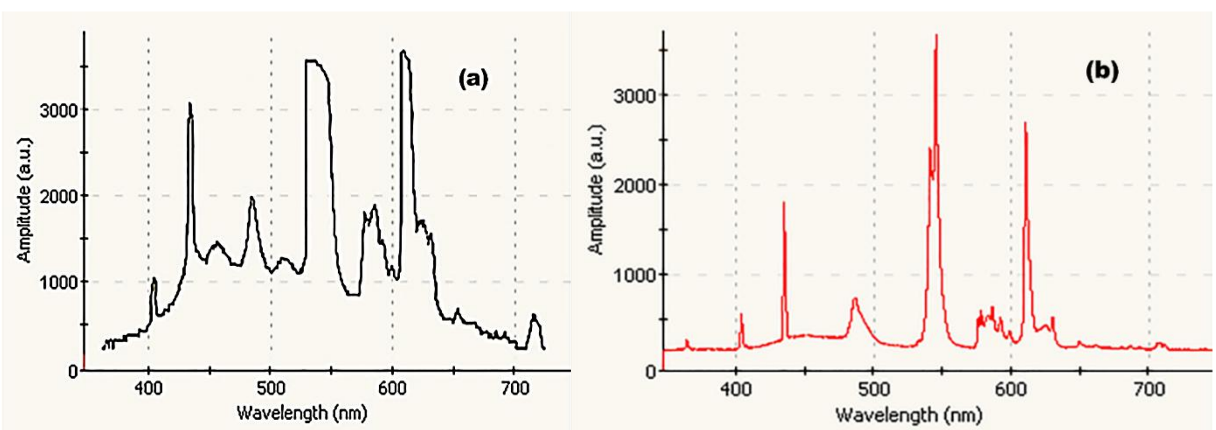

Figure 6. Spectrum of a common CFL lamp emission taken by (a) presented spectrometer (b) ocean optics commercial spectrometer.

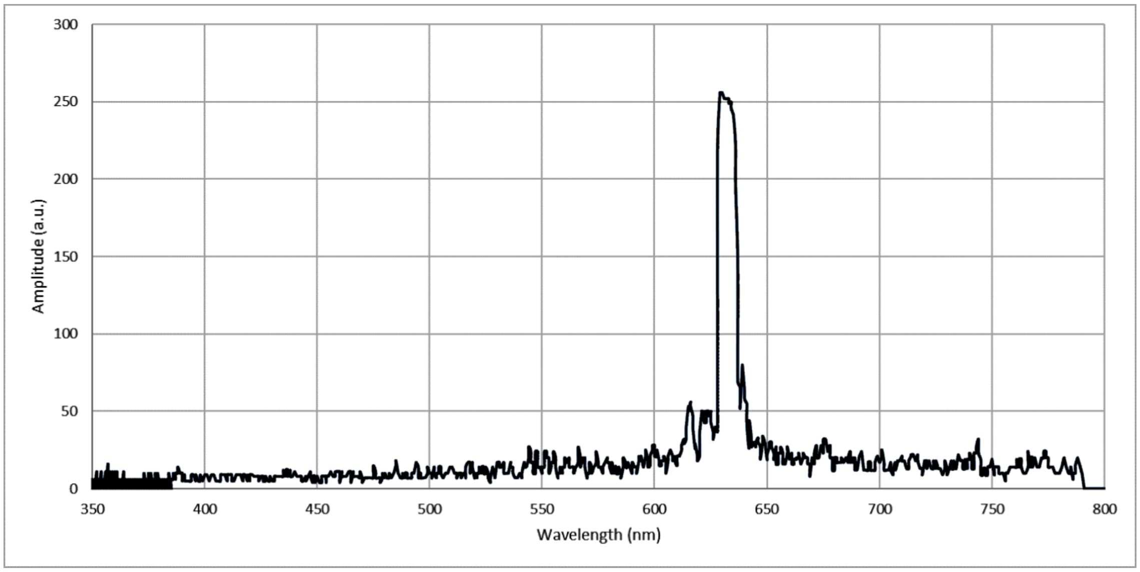

Figure 7. Spectrum of a 630 nm laser diode emission.

As the datasheet indicates, moderate dynamic range of the CCD sensor hinders the sensitivity of the device for low-intensity lights source spectra by raising the dark signal introducing more noise to the spectral data. This is undesirable for an application such as Raman spectroscopy, which produces a very weak photon emission as the Raman spectrum. The sensitivity may be raised by the use of a better CCD sensor which has a higher dynamic range and properly shielding the analogue circuitry from digital noise. The ADC can be also upgraded for better resolution and probable noise reduction. Reducing the photo element temperature is yet another approach that can be used to reduce background noise and was developed as an extension to be added to this instrument. The effect of the thermoelectric cooler on the dark current of the CCD is evident in Figure 8.

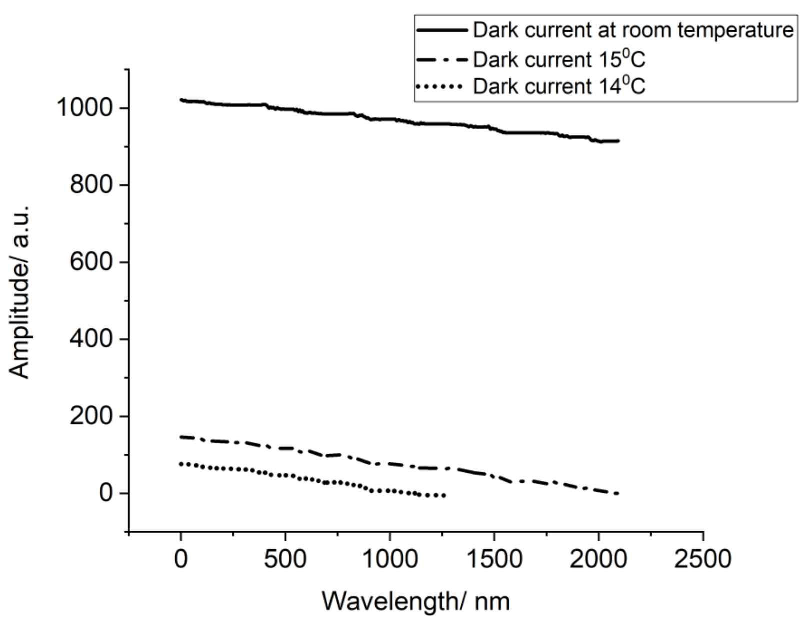

Figure 8. The reduction in dark current with a reduction in the CCD temperature.

The main goal of this work was to design and construct a portable USB driven spectrometer which can achieve the results that are compatible with commercially available spectrometers but at a much lower cost.

The spectrometer and application software adequately performs well given that the input radiation has sufficient intensity. Considering the low price point (<USD 250), accuracy and resolution of a wavelength and amplitude calibrated spectrum is reliable.

The spectrometer is well-suited for undergraduate and high school laboratory experiments and demonstrations, as well as field-based research work which do not require a high degree sensitivity.

In order to upgrade the spectrometer to a device with high sensitivity as in the case of Raman spectroscopy, the main limiting factor was identified to be the dynamic range of the CCD. A back-thinned CCD with a high dynamic range (≈125,000) and high quantum efficiency is required for the operation of a Raman micro-spectrometer.

Acknowledgement

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