Spectral Laser Elemental Analyzer

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Abstract — This paper presents the design practices used to create a low-cost portable LIBS system. The prototype is used for the identification and analysis of non-organic samples. Developed by a multidisciplinary undergraduate team, the system ensures consistent plasma generation, minimal measurement variance, and accurate identification of alloys. The system uses an Nd:YAG laser to generate plasma. A Czerny-Turner spectrometer in conjunction with a linear CCD for diffraction and spectral analysis, and an MCU for data processing and transmission. . Through market investigation and technology comparison, the system adheres to safety standards while maximizing functionality. Addressing challenges in hazardous and extraterrestrial environments, this project showcases the potential of Laser-Induced Breakdown Spectroscopy for diverse applications beyond terrestrial exploration.

Index Terms — LIBS, spectral analysis, Nd:YAG laser, Czerny-Turner, Linear CCD, MCU.

INTRODUCTION

The SpectraLaser Elemental Analyser is the undergraduate senior design project of UCF's College of Electrical Engineering and Optics and Photonics. The team members are Liam Collins, Benjamin Logan, Faisal Abdullah Salim Al-Quaiti, and Stephen Styrk. The objective of the project was to create a LIBS system that can have applications in hazardous environments, extraterrestrial exploration, or educational institutions. The SpectraLaser Elemental Analyser provides a lower cost alternative to the highly expensive LIBS systems currently on the market. This project involved designing, building, and testing all of the electrical and optical systems that are required to form a LIBS system.

STANDARDS & CONSTRAINTS

The industry standards and guidelines that related to this project include: General requirements (29 CFR 1910.132), along with the eye and face protection (29 CFR 1910.133) requirements. There are additional voluntary guidelines which are provided by the American National Standards Institute (ANSI). The ANSI guidelines related to the project are: Safe Use of Lasers (Z136.1), Recommended Practice for Laser Safety Measurements for Hazard Evaluation (Z136.4), Safe Use of Lasers in Educational Institutions (Z136.5), Safe Use of Lasers Outdoors (*Z136.6*). The electrical standards relevant to this project included IEC61010, covering safety requirements of electrical equipment for measurement, control, and laboratory use. IEC60812 systematic evaluation of hardware, software and other processes. IPC-2221, and IPC-2222 are the sets of standards that cover the dimensions, designs, and other aspects of PCBs which would be used in the project. For the spectroscopy optical systems The U.S. Military Performance Specification MIL-PRF-13830B and ISO 10110 are two standards that help identify the needs of the system with regards to surface quality specifications.

The constraints that were relevant to this project include: Safety, Supplier Limitations, Cost, and Time. Safety is a major constraint of the LIBS project. Laser induced breakdown spectroscopy requires a powerful laser to atomize the material and create plasma for the spectrometer to measure. Without proper safety procedures in place it is possible that the laser could cause eye damage to bystanders during testing. A containment unit was created to fully enclose the laser. This ensures that no laser excitation light escapes, which will ensure eye safety of users and bystanders.

OPTICAL SYSTEMS

The two primary optical systems designed are the laser that will create plasma and the spectroscopy system.

LASER DESIGN & SELECTION

The laser used for this project needed to be able to create plasma from inorganic materials consistently and in a safe manner. The laser selected is a 1k Watt laser designed for tattoo removal. This laser has the required intensity to create plasma. Using the specifications of the laser provided in table 1 we can show that the laser is able to create plasma as the Irradiance (or Peak Power) is greater than 10^8 W/Cm^2 .

$$\text{Peak Power} = \text{Pulse Energy} / \text{Pulse Width} = \frac{0.3\,\mathrm{J}}{8\times10^{-9}\,\mathrm{s}} = 37.5\times10^{6}\,\mathrm{W}$$

$$\text{Peak Power Density} = 0.05\times10^{-4}\,\mathrm{m}^2 \,/\, 37.5\times10^{6}\,\mathrm{W} = 7.5\times10^{14}\,\mathrm{W/m}^2$$

The focal length of the focusing system for the laser is 100 mm from the laser emission point. This helps mitigate any debris issues that might affect optical components. The laser focusing system uses a Telephoto lens design to extend the focal point. The laser bought has a lens t

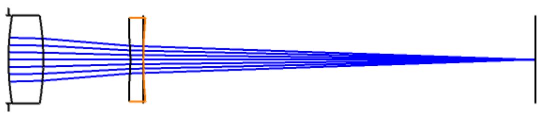

Fig.1 ZEMAX visual

	Surface Type		Comment	Radius	Thickness	Material	Coating	Clear Semi-Dia		Chip Zone	Mech Semi-Dia	Conic	TCE x 1E-6
0	OBJECT	Standard		Infinity	Infinity			0.000		0.000	0.000	0.0...	0.000
1	STOP	Standard		Infinity	0.000			10.000	U	0.000	10.000	0.0...	0.000
2	(aper)	Standard	L1S1	60.990	8.000	N-BK7		10.000	U	0.000	10.000	0.0...	-
3	(aper)	Standard	L1S2	-60.9...	20.000			10.000	U	0.000	10.000	0.0...	0.000
4	(aper)	Standard	L2S1	-50.0...	3.000	N-BK7		9.000	U	0.500	9.500	0.0...	-
5	(aper)	Standard	L2S2	100.0...	0.000			9.000	U	0.500	9.500	0.0...	0.000
6		Standard	Focal Point	Infinity	89.995			10.000	U	0.000	10.000	0.0...	0.000
7	IMAGE	Standard		Infinity	-			10.000	U	0.000	10.000	0.0...	0.000

Fig.2 ZEMAX code

The laser selected has the following parameters that will be meeting the needs of the project.

Power	1000 W
Frequency	1-10 Hz
Power Supply	110 V
Pulse Energy	Single Pulse ≥ 160 mJ, Double Pulse ≥ 270 mJ, Multi-pulse ≥ 700 mJ
Spot Area	1-5 mm
Laser House/Cooling	49x32x31cm
Pulse Width	8 ns

Table 1

Back reflections were another concern with the laser focusing design. However using Ray Optics simulation for the selected lenses at their described distances showed that any back reflections would not damage the components.

SPECTROMETER DESIGN

The design for the spectrometer was a crossed Czerny-Turner configuration. This provides high spectral resolution, minimized stray light, superior collimation and focus in a compact system. The system will be observing the visible spectrum, 380 nm to 700 nm, from the plasma created by the laser system. For elemental characterization it is desirable to have a high spectral resolution. The geometry selected for the Czerny-Turner is $\phi = 30°$. This strikes a good balance between diffraction efficiency and minimizing aberrations in the system. The grating of the system was chosen for peak efficiency, G = 1200 lines/mm. This provides a blaze wavelength of 500 nm. This is in the middle of the observed visible spectrum. The chosen linear CCD has a width of $L_D = 28.6\ mm$. The proposed spectrometer will be using a 905-fiber cable with a collimating lens attached to the end to guide the light to the spectrometer.

Based on these choices the angle of incidence (3), diffraction angle (4), focal length of the focusing mirror (5), focal length of the collimating mirror (6), and slit width (7) were calculated. The results of these calculation are located in table 2

$$(\lambda_2 - \lambda_1) = \lambda_R \qquad (1)$$

$$\frac{\lambda_R}{2} = \lambda_C \qquad (2)$$

$$\alpha = \sin^{-1}\left[\frac{\lambda_C G}{2\cos(\frac{\phi}{2})}\right] - \frac{\phi}{2} \qquad (3)$$

$$\phi = a + B \qquad (4)$$

$$L_F = \frac{L_D \cos(\beta)}{G(\lambda_2 - \lambda_1)} \qquad (5)$$

$$L_C = \frac{L_F \cos(\alpha)}{M\cos(\beta)} \qquad (6)$$

$$W = \frac{G\,\Delta_{\lambda} L_C}{\cos(\alpha)} \qquad (7)$$

The spectrometer has changed slightly from the original planning and design. I have replaced the focusing mirror with a mirror that has a 100 mm focal length. This helped to create a proper crossed Czerny-Turner style spectrometer and to more easily allow for the positioning and alignment of the system. This will have no effect on the overall system resolution.

Minimum wavelength	λ_1	380 nm
Maximum wavelength	λ_2	700 nm
Wavelength range	λ_R	320 nm
Center wavelength	λ_c	540
Detector width	L_D	28.6 mm
angle of incidence	α	$14.98°$
diffraction angle	B	$44.98°$
focusing mirror focal length	L_F	$52.66\ mm$
collimation mirror focal length	L_C	$70\ mm$
slit width	W	$28.6\ \mu m$

Table 2

SPECTROMETER RESOLUTION

Since this is a dispersive array spectrometer, three optical components are the main factors in determining spectral resolution, the most important aspect of a spectrometer. The slit, diffraction grating, and the detector contribute to the systems overall ability by determining the maximum number of spectral peaks that the spectrometer can resolve. The slit will determine the minimum image size formed on the detector, the diffraction grating determines the total wavelength range of our spectrometer, and the detector determines the maximum number and size of discrete points that can be digitized. The spectral resolution $\delta\lambda$ is calculated with equation (8). The results of this calculation can be seen in table 3.

$$\delta\lambda = \frac{RF*\Delta\lambda*W_s}{n*W_p} \qquad (8)$$

The Spectral resolution is determined by the FWHM. The resolution factor requires at least 3-pixel width to determine FWHM, if $W_s \approx 2W_p$ then the resolution factor drops to 2.5. The slit purchased is 25 μm +/- 2 μm . The calculations remained at the designed values since this small difference has a negligible impact on the overall system.

Spectral Resolution	$\delta\lambda$	0.997 nm
Resolution factor	RF	2.5
Slit width	W_s	28.6 μm
Spectral range	$\Delta\lambda$	300 nm
Pixel width	W_p	14 μm
Number of pixels	n	2048

Table 3

ELECTRICAL SYSTEMS DESIGN

The electrical systems designed for the system are split into two parts. The electrical control and sensing systems along with the power systems. The control and sensing systems dealt with detecting when the laser was triggered, driving the CCD along with capturing its output results, and transmitting those results to an external machine. The power subsystems dealt with supplying power to the control and detection systems.

ELECTRICAL CONTROL AND SENSING SYSTEMS

The electrical control systems are composed of three subsystems. The laser blast detection system, Spectral Emission Measurement Subsystem, and Data Output Subsystem. The MCU that interfaces with each of these subsystems is the STM32G474RET6. This MCU operates at up to speeds of 170 MHz, uses a 3.3V supply for power, and provides sufficient timers and I/O resources for the system. This MCU also offers a 12-bit ADC and native USB support, along with 128 KB of RAM for sample data set storage. The overall block diagram for the electrical control and sensing systems can be seen in figure 3.

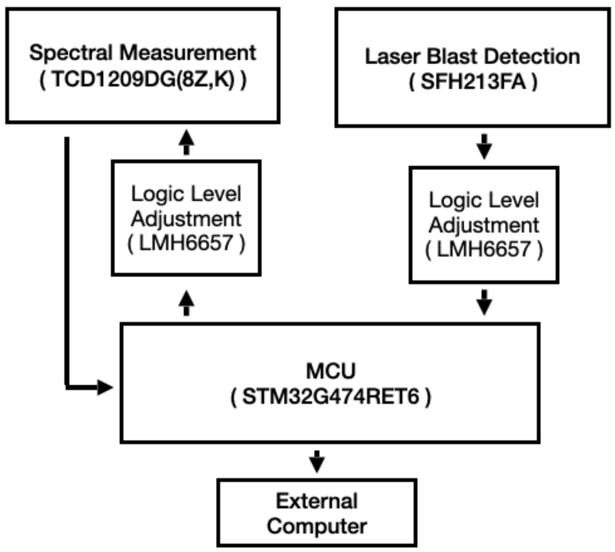

Fig.3 Electrical control & sensing systems block diagram

Laser blast detection subsystem

The laser blast detection sub-system is used to determine when the laser has been fired and outputs a signal to the MCU when firing occurs. The MCU uses this signal to trigger the timing for driving the CCD and capture results at the appropriate time. A block diagram of the subsystem can be seen in figure 4.

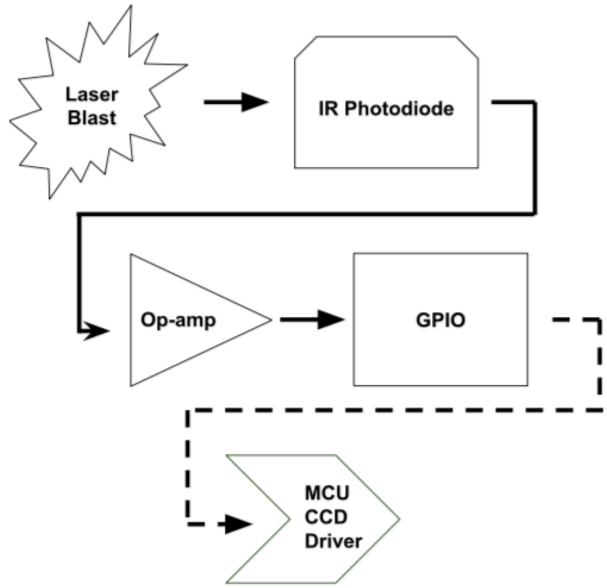

Fig.4 Laser blast detection subsystem Block diagram

The laser blast detection circuit uses a photodiode to detect the laser blast, an op amp compares the output voltage of the photodiode with a set reference voltage. The op amp triggers a signal of the appropriate logic level to one of the MCU's GPIO pins when the output voltage of the photodiode exceeds the op amp's reference voltage. This triggers the CCD's capture sequence. The photodiode chosen for this subsystem is the SFH213FA. This photodiode was chosen for its fast response time, which was listed as being on the order of tens of nanoseconds. The photodiode is biased at 5V to aid its reaction time to the laser blast. The LMH6648MAX op amp was chosen to compare the output of the photodiode with a set reference voltage. This op amp was chosen due to its high slew rate of 420 V/us, which allowed for rapid output responses to the MCU when changes occurred in the photodiode. The reference voltage for this circuit was created with two resistors to form a voltage divider. The reference voltage was set to 2.2 V, this value was selected based on testing. This circuit also allows the sensitivity of the comparator to be adjusted based on the resistors, which provides a level of flexibility for tuning the design. The schematic for the design of this subsystem can be seen in figure 5.

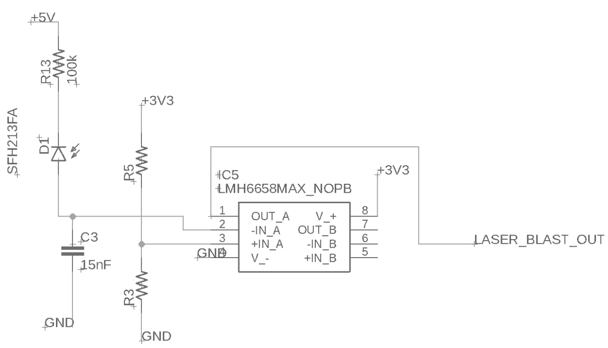

Fig.5 Laser blast detection subsystem schematic

Spectral emission detection subsystem

Spectral emission detection subsystem consists of the Linear CCD which catches the refracted light output from the diffraction grating of the spectroscopy system. Op amps are used as level shifters to translate the logic levels of the MCU's 3.3V control signals to the 5V logic level used by the CCD inputs. An ADC is used to convert the analog output of the CCD to digital form for processing by the MCU. The block diagram of the Spectral emission detection subsystem can be seen in figure 6.

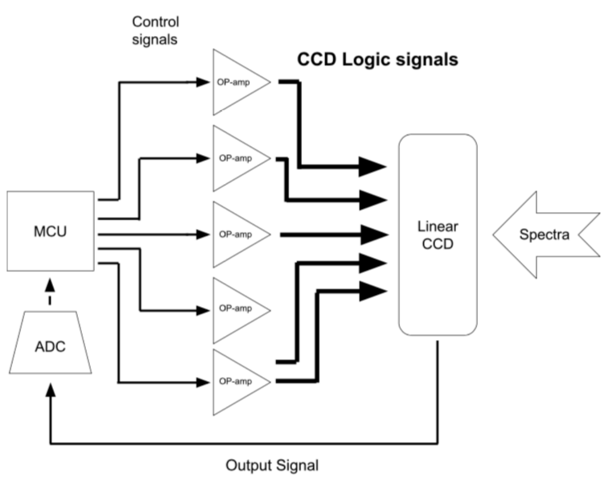

Fig.6 Spectral Emission Measurement Subsystem Block Diagram

The CCD selected for this design is Toshiba's TCD1209DG(8Z,K). This CCD was selected for its high dynamic range, relative to other CCDs in the same price range. The high dynamic range of this CCD allows for greater ease of differentiating different peaks and valleys in the emission spectra of samples. This CCD is powered by a 12V supply, and is driven by five control signals, which require 5V logic. These control signals reset the CCD at the beginning of the capture sequence and control the speed at which the discrete photo detection elements are shifted to the analog output. The CCD has a total of 2087 photo detection elements, of which 2048 provide true results for light intensity measurements. Each of these elements are sequentially shifted to the output of the CCD during a single integration or measurement period. The CCD has a maximum frequency of 20MHz.

The LMH6648MAX op amps were chosen for level shifting the 3.3V logic of the MCU's control signals to the 5V required to drive the CCD. Op amps were chosen over traditional level shifter ICs, as they provided an added level flexibility on a per signal basis. The op-amps that were chosen have a sufficient slew rate to ensure that they can switch quickly enough to drive the CCD up to 20MHz. This op amp easily allows the CCD and MCU to operate in tandem. A voltage divider was used as the reference voltage for these op amps. The reference voltage was set at around 1.8V, this value was chosen based on test results. The analog output voltage of the CCD is captured by the MCU's internal ADC. The schematic for this subsystem can be seen in figure 7

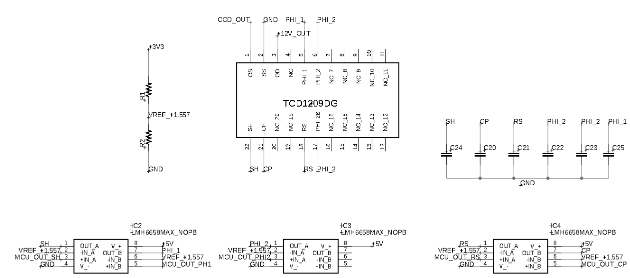

Fig.7 spectral emission detection subsystem schematic

Data output subsystem

Spectral data captured by the CCD is stored in the MCU. The data is held there until it is output to an external machine via a USB connection. The STM32G474RET6 MCU offers native USB support, and provides data plus and data minus pins directly on the IC. The output subsystem uses these differential data plus and data minus USB pins to directly connect to an external machine. The block diagram for this subsystem can be seen in figure 8.

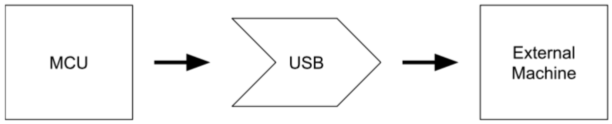

Fig.8 Data output subsystem block diagram

Decoupling capacitors were added to the differential data lines to provide noise reduction. However correct information was capable of being transmitted without any capacitors present on the data lines. The schematic for this subsystem can be seen in figure 9.

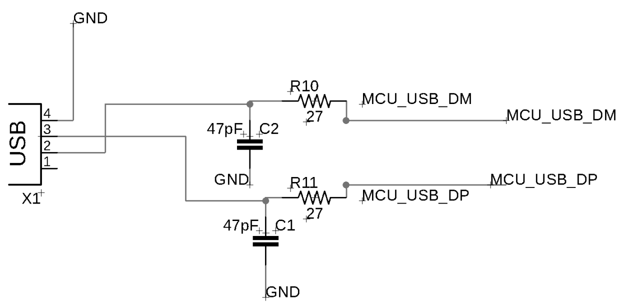

Fig.9 Data output subsystem schematic

POWER SYSTEMS

The power systems of the design are used to supply power to all of the electrical systems except the laser, which was powered by its own separate supply. The MCU requires a 3.3V supply, while the CCD needs both 5V inputs and a 12V supply. Two switching regulator circuits were designed to supply the MCU and CCD Inputs with their required voltages. A block diagram of the overall power systems of the design can be seen in figure 10.

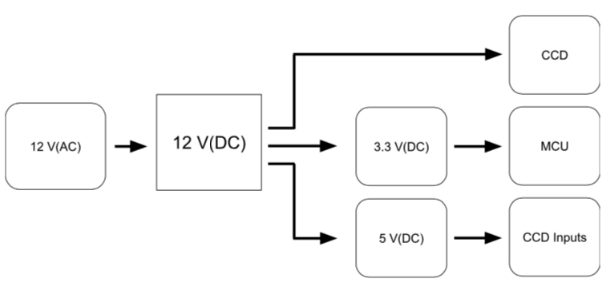

Fig.10 Power systems Block Diagram

The design of the power systems is based on the projected maximum power requirements of all the combined system components. Based on the information provided by the data sheets of the various devices, it was determined that no more than 500mA at most would be required by all of the devices simultaneously. Therefore the power systems were tailored to be capable of providing up to 500mA.

The MCU is supplied with its required 3.3V by the LMR50410 IC. This circuit will function with input voltages between 10V and 13V. The operating frequency of the LMR50410 is 700KHz. The schematic for this regulator circuit can be seen in figure 11.

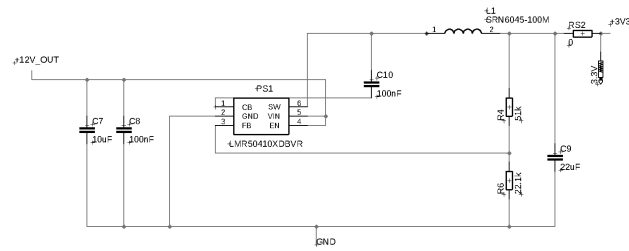

Fig.11 3.3V regulator schematic

The LMR54406 supplies the operational amplifiers that translate the MCU control signals from 3.3V to 5V for the CCD. The operating frequency of the LMR54406 is 1100KHz.The schematic for this regulator circuit can be seen in figure 12.

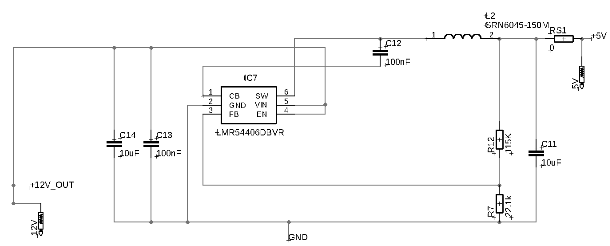

Fig.12 5V regulator schematic

The 12V supply required for the CCD was provided directly from the 12V wall transformer, which also supplied the regulator circuits.

SOFTWARE

The software for the design is split into two areas. The firmware for the MCU which was written in C, and the software for the external machine which was written in python.

MCU FIRMWARE

The MCU used in this design is the STM32G474RET6. ST provides many of its own API’s and functions to operate the various peripherals on the ST chips. These features can alleviate the more tedious aspects of initializing and starting various functions on the chip. However these functions and API's can fall short due to overhead, when high amounts of speed or precision are required. In those cases directly accessing the chip's registers was more fruitful. The chip was programmed using ST's CUBEIDE software, along with the ST-link and the STM32's single wire debug pins.

The overall block diagram of the MCU's software loop can be seen in figure 13.

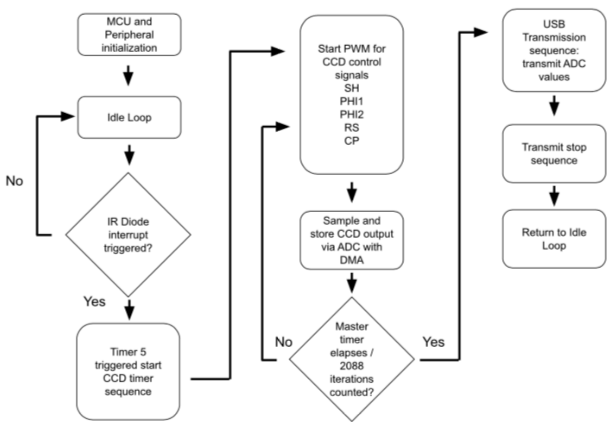

Fig.13 Overall MCU control flow

The MCU idles until the laserblast triggers the start of the CCD capture sequence. At which point the various control signals to the CCD run allowing all 2087 CCD elements to be sampled by the ADC. The sample data is then transferred to the external machine.

CCD control signal organization

One of the primary reasons that this MCU was used, was it provides an abundance of complex PWM timers. These timers are necessary to properly drive the five inputs to the CCD. The control signal diagram provided by Toshiba for the CCD can be seen in figure 14.

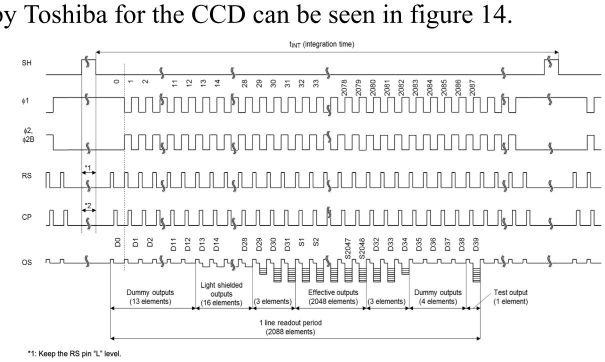

Fig.14 CCD timing diagram

This diagram along with the timing restrictions of each signal needed to be matched by the output waveforms from the MCU. This required syncing the timers together by having timers trigger other timers. The overall triggering arrangement can be seen in figure 15.

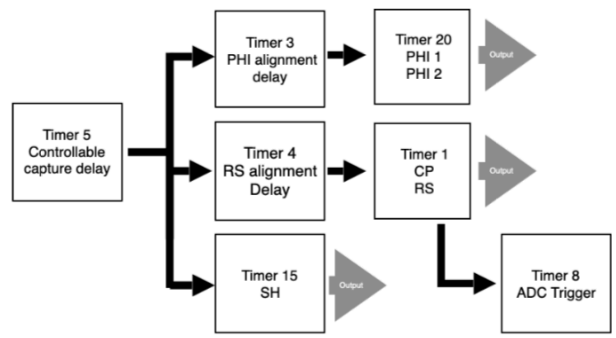

Fig.15 Timer triggering sequence

Timers were used for creating the CCD control signal waveforms on the GPIO pins of the MCU, as low level GPIO register manipulation proved too slow for the system's desired speeds. Signal jitter was also less apparent in synced output timer signals when compared with GPIO or Direct Memory Access methods for output waveform generation. This timer sequence was triggered by an external GPIO pin on the MCU that was connected to the output of the laser blast detection circuit.

There was a very small window for the ADC to perform its conversion on each of the CCDs light sensing elements, as they are clocked to the CCD's output. Timer 8 was used to trigger the MCU's ADC in the correct window of time to capture the correct data.

The max clock speed of the MCU's internal ADC is 60 MHz. At a resolution of 12-bit, 12.5 clock cycles are needed to complete a sample and hold period(T_{SAR}) of the ADC. Therefore the time for the ADC to perform a conversion is calculated with equation (9).

$$t_{convert} = \frac{T_{SAR}}{F_{ADC}} \qquad (9)$$

At 12-bits the ADC has a delay of 209ns. This means that with the MCUs internal ADC the maximum speed that the CCD can be driven at is around 4MHz, with an integration time of 437 μs to account for all 2087 elements. The CCD was set to run at around 2MHz, resulting in an integration time of close to 1ms. This is well within the expected range of integration times based on work done by others[1].

Data transmission sequence

Data is transmitted from the MCU by using the internal USB support for the MCU, provided by ST. The MCU sets up a virtual COM port. This COM port is then used to transmit the stored CCD serial data to the python program on the external machine. The MCU offers full speed USB support.

EXTERNAL MACHINE SOFTWARE DESIGN

The software for the external machine is written in Python. Python easily allows for the ability to organize and graph the spectral data. The python package 'pyserial' is used to read the USB outputs from the MCU's virtual comport, and store the data. The data received from the MCU is parsed into its separate CCD elements. The primary control loop for the external machine software can be seen in figure 16.

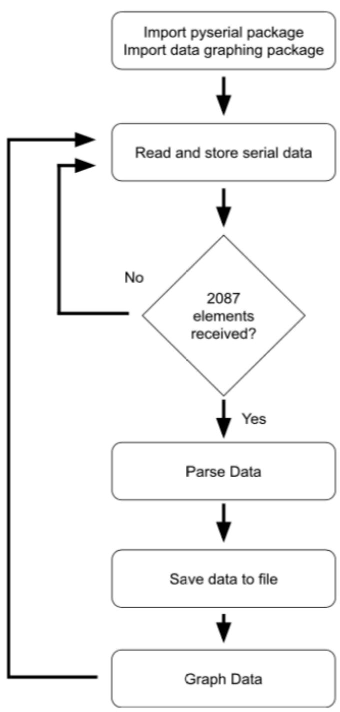

Fig.16 External machine control flow

The Python program idles until the pyserial package detects that all 2087 elements have been received from the MCU. Once transmission has been completed, the data is parsed to split it into its individual elements. The pandas package is then used to establish a dataframe to store all of the individual CCD elements. The data frame is then saved to a .csv file with a unique name and time. The plotly package is then used to graph the data in an interactive HTML window for display.

PCB DESIGN

The PCB created for this design uses a six layer stackup of Signal-Ground-Power-Power-Ground-Signal. A ground trace was added alongside the signal trace of the CCD's analog output. This trace along with the two ground plates were added to help reduce noise on the PCB. This idea was based on the work of Dr.Eric Bogatin who teaches Practical PCB design and the Senior Design courses at the University Colorado Boulder. A 5V and 3.3V power power plane were added to the design based on the recommendation of Dr.Arthur Weeks. The PCB is fully functional, and all electrical subsystems work correctly.

ACKNOWLEDGEMENTS

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Citations

[1] Emanuela Grifoni, Stefano Legnaioli, Marco Lezzerini, Giulia Lorenzetti, Stefano Pagnotta, Vincenzo Palleschi, "Extracting Time-Resolved Information from Time-Integrated Laser-Induced Breakdown Spectra", Journal of Spectroscopy, vol. 2014, Article ID 849310, 5 pages, 2014. https://doi.org/10.1155/2014/849310

[2] Robert Feranec. Do You Really Need Power Planes? Are you sure? | Eric Bogatin. (Nov 20, 2021). Accessed: Jan. 24, 2024. [Online video]. Available: https://www.youtube.com/watch?v=kdCJxdR7L_I