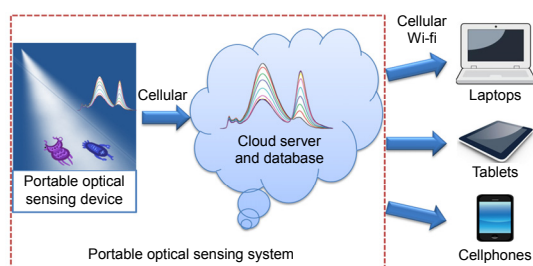# A portable optical sensing system for rapid detection of fluorescence spectra

Xiaoguang Li[1], Haoyu Yu[2], Yuenkeong Yew[3],

Hongzhong Liu[2] and Minghui Hong[3]*

[1] Xi'an Microelectronics Technology Institute, Xi'an 710119, China;

[2] State Key Laboratory for Manufacturing Systems Engineering, Xi'an Jiaotong University, Xi'an 710049, China; [3] Department of Electrical and Computer Engineering, National University of Singapore, 4 Engineering Drive 3, Singapore 117581, Singapore

Abstract: Development of a prototype of a portable optical sensing system is presented for fast detecting of samples' fluorescence spectra. A compact configuration is achieved by integrating a small spectrometer, a microcontroller, a Universal Serial Bus (USB) Host Shield, a network module, and a web server. The fluorescence spectra of a tested sample can be obtained. Then the test data are sent through network communication to our Cloud Server which can store the data for further analyses. With this configuration, test results can be revealed in a short time and downloaded by users to their laptops, tablets or cellphones anytime and anywhere.

Keywords: optical sensing; real-time detection; fluorescence spectra

1 Introduction

Fluorescence is the emission of light from a substance that absorbs electromagnetic radiation [1]. When certain atoms are irradiated with the electromagnetic radiation (usually in the form of light), the energy of the radiation causes some electrons around the nucleus to transit from the original orbit to the higher energy orbit, from the ground state to the excited singlet. The singlet is unstable and the electrons tend to transit back to the steady state. When the electron is restored from the excited singlet state to the ground state, the energy is released in the form of light, resulting in fluorescence. In most cases, the emission light has a longer wavelength, and possesses lower energy than the absorbed radiation. However, when the absorption intensity is strong, a two-photon absorption phenomenon may occur, resulting in a shorter radiation wavelength than that of the absorption light. The fluorescence is a form of photoluminescence, and the radiation materials cease to glow immediately when the radiation source stops [2]. The most striking example of fluorescence is the absorbed radiation in the ultraviolet region of the spectra which is invisible to the human eyes, while the emitted light is in the visible region and gives a distinct color.

Fluorescence has a wide variety of applications, including gemology, mineralogy, medicine, chemical sensing, printing dye, and biological labellings [3-6]. Detection methods based on spectral analysis techniques are an interesting alternative for performing sensitive, selective and reliable measurements. The application of fluorescence in spectral analysis is fluorescence spectrometry which has been successfully employed as a basic measurement method to obtain the characterization of chemical constituents for food classification, water pollution, bacterial pathogens detection and plant species characterization. It has the advantage of minimal sample preparation and relatively low-cost instrumentation [7-11]. Much effort has been done to improve the performance of the fluorescence spectral analysis devices to increase precision and speed [12, 13]. Though various methods have been explored to improve the instruments' design and manufacture, portability remains a huge challenge.

This paper provides the details regarding the fundamental of a portable optical sensing system to rapidly detect the fluorescence spectra of the testing samples. The system integrates a suitable spectrometer as an optical sensor and a microcontroller to execute all instructions, which offers a potential solution to resolve the portability and performance. Meanwhile, several modules have been added to enable functionalities, such as image capture,

wireless transmission and location tracking. Experimental results on several water samples show the capability of our prototype as a smart tool.

2   System implementation

The concept of the portable real-time optical sensing system is illustrated in Fig. 1.

This system is aimed to rapidly detect fluorescence spectra within a compact configuration. Besides the basic hardware for sensing and sending results, a database in the cloud environment is also adopted for data storage. Firstly, the spectrum of a tested sample can be obtained by the portable optical sensing device. Then the data is sent through network communication to the Cloud Server. Since the cloud storage technique is employed, users can download the results to their laptops, tablets or cellphones anytime and anywhere.

2.1   Hardware framework

The hardware capabilities of the system include acquiring spectra, taking pictures, acquiring locations, and sending data to the web server. The main components include a spectrometer (Ocean Optics), a Microcontroller Board (Arduino), a USB Host Shield (Arduino), a Third-Gene-

ration + Global-Positioning-System (3G+GPS) Shield (3E Gadgets) and a Webserver (Amazon), which are shown in Fig. 2. In working condition, the Arduino microcontroller first initializes the USB650 Spectrometer, through the Arduino USB Host shield. Then it sends commands to the spectrometer to acquire the spectra of the sample. Through the GPS system, the microcontroller acquires the location of the sample taken and captures a picture of the collected sample using Hayes command sets (AT command). Next, together with the spectra data, the microcontroller sends this information to the web server through the 3G network using 3G + GPS shield for Arduino. In the final step, the web server categories and processes the spectra data by linking it to the database. The analyzed results are returned to the web server for users to view from any mobile devices that have web browsers, by logging into the web server.

2.1.1 Spectrometer as optical sensor

In prototyping the optical sensing system, Ocean Optics Red Tide USB650 spectrometer was selected as the sensor. It offers real-time capturing full spectra ranging from wavelength 350 nm to 1000 nm in 25 milliseconds [14]. The spectrometer connects to a computer via a USB port, drawing power from the host, thus eliminating the need
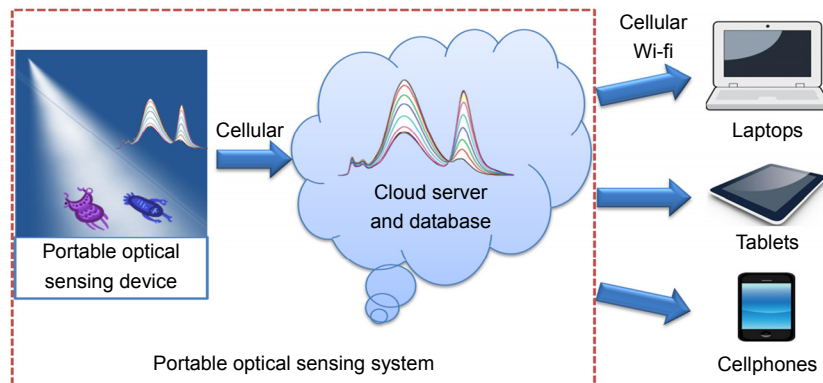

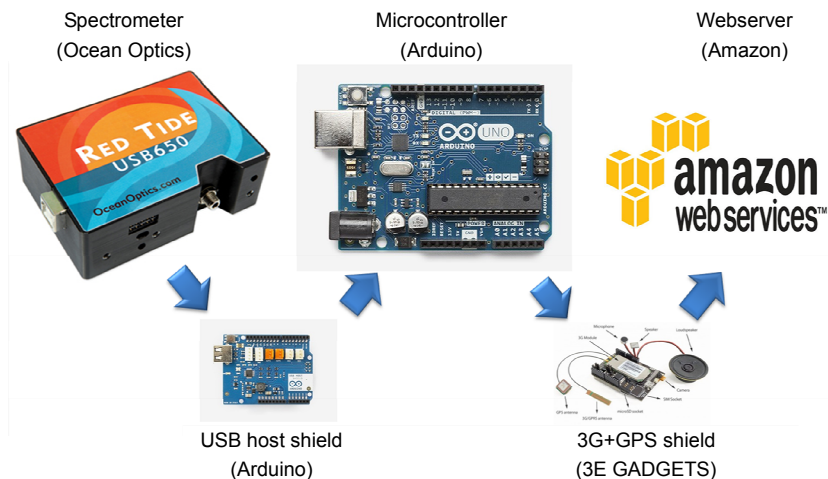Fig. 1   Real-time optical sensing system implementation.

Fig. 2   The main components of the system's hardware.

for an external power supply. In addition, the USB650 has an optical resolution of 2.0 Full Width Half Maximum (FWHM) at 2 nm, which implies a moderate detecting capability. The cost of USB650 is one of the lowest in the family of spectrometers, and it could be interfaced to communicate with other peripherals. Since no built-in light source is contained, it is linked up with a light source to obtain fluorescence spectra of the samples (532 nm central wavelength).

2.1.2 Microcontroller

The Arduino Uno is easy to be used in powerful single board based on ATmega328P microcontroller with the throughput of 20 MIPS (million instructions per second) at 20 MHz [15]. The Arduino is open-source, which means the hardware is reasonably priced and development software is free. Thus, it has gained considerable attention.

The Arduino UNO board can be programmed in the following phases: (i) setup phase, and (ii) execution phase. In the setup phase, the USB host shield, USB650 spectrometer, 3G + GPS shield are sequentially initialized. Firstly, the USB host shield is initialized to establish communication with the USB650 spectrometer. Then the spectrometer will be initialized and followed by the 3G+GPS shield. During this period, the camera, as well as the SIM5218 network communication module, is initialized. The microcontroller will then proceed to execution phase once all these modules are checked.

In the execution phase, the microcontroller will start to call the function, "Acquire_Spectra()", to acquire spectra data by setting the trigger mode, integration time and enable strobe light of the spectrometer. Then the function "Take_Picture()" will capture an image of the sample, and determine the location where the sample was collected by calling "Locate_Position()" and finally, the function "Send_to_Webserver()" will send these data to the Amazon web server.

2.1.3 USB host interface

The Arduino USB Host Shield, when configured, allows connections of any USB devices to the Arduino microcontroller board. This interface shield consists of an MAX3421E USB host controller, which contains digital as well as analog circuitry capable of implementing a full-speed USB compliant to USB Specification Rev 2.0 which supports 60 MB/s transfers. In addition, it is also a microprocessor independent USB because the MAX3431E controller makes vast collection of USB peripherals available to any microprocessor. Hence for a point-to-point connection, in this case, the real-time optical system, and the firmware to establish communication can be simple since only a targeted device, USB650 Spectrometer, is supported.

When the USB650 spectrometer is first connected to the USB Host Shield, the USB enumeration process begins. The Host resets the USB650 and requests for the Device Descriptor. A new address will be set upon the response of the spectrometer to the host. Then the host

reads the .INF file and specifies the driver. The host selects configuration once the driver is loaded. The real-time system adopts a Control Transaction type of USB communication protocol. There are three simple steps to establish communication: identify, configure and control device. When the spectrometer is connected to the Arduino USB Host, the host requests information from the spectrometer, such as capability and power requirement. In return, the spectrometer will provide this information back to the host in a form of a description table. This description table has a structured sequence of values defined by the developer. The device descriptor gives the host vital information like Vendor Identification (VID) and Product Identification (PID) that are crucial for the programmers to configure and interface with the system.

The program codes to configure the USB650 spectrometer are simple. Upon the detection of the USB650 spectrometer, the function "Usb.getDevDescr()" is called to get the device descriptor. Next, the Vendor Identification and Product Identification are checked. If they match, the attributes obtained in the device descriptor will be set by calling "Usb.setEpInfoEntry()". Next, the function "Usb.setConf()" will be called to set the configuration of the USB650 device. Upon the completion of the USB configuration, the first command is sent out by calling the function "Usb.outTransferQ" to initialize the USB650 spectrometer. Finally, the USB state is set to be running state through the function "Usb.setUsbTaskState (USB_STATE_RUNNING)".

2.1.4 Network communication module

Once the microcontroller is determined, the search for the suitable communication module or shield will also be determined. The system adopts the GPS shield for Arduino. This communication module comes with an internal GPS that enables the location of the devices outdoor or indoor using both assisted-mobile (A-GPS) and mobile-based (S-GPS) modes. The module comes with a video camera, which enables the recording of video or photos capturing in high resolution of 640 pixels×480 pixels. Most importantly, this communicating module is designed to work with Internet servers implementing several internally application layer protocols, which make it easier for cloud communication, such as Hypertext Transfer Protocol (HTTP) and Hypertext Transfer Protocol Secured (HTTPS) navigation. Similarly, the module provides File Transfer Protocol (FTP) and File Transfer Protocol Secured (FTPS), thus making it easier for file handling. Lastly, the communication module has a Micro Secure Digital (SD) slot that can store data up to 32 GB.

2.1.5 Webserver

The portable optical sensing system uses the Amazon Elastic Compute Cloud (EC2) as a web service to store spectra data, sample pictures as well as GPS data. It provides a sizeable computational capacity in the cloud with a storage space up to 30 GB and 750 hours of free usage
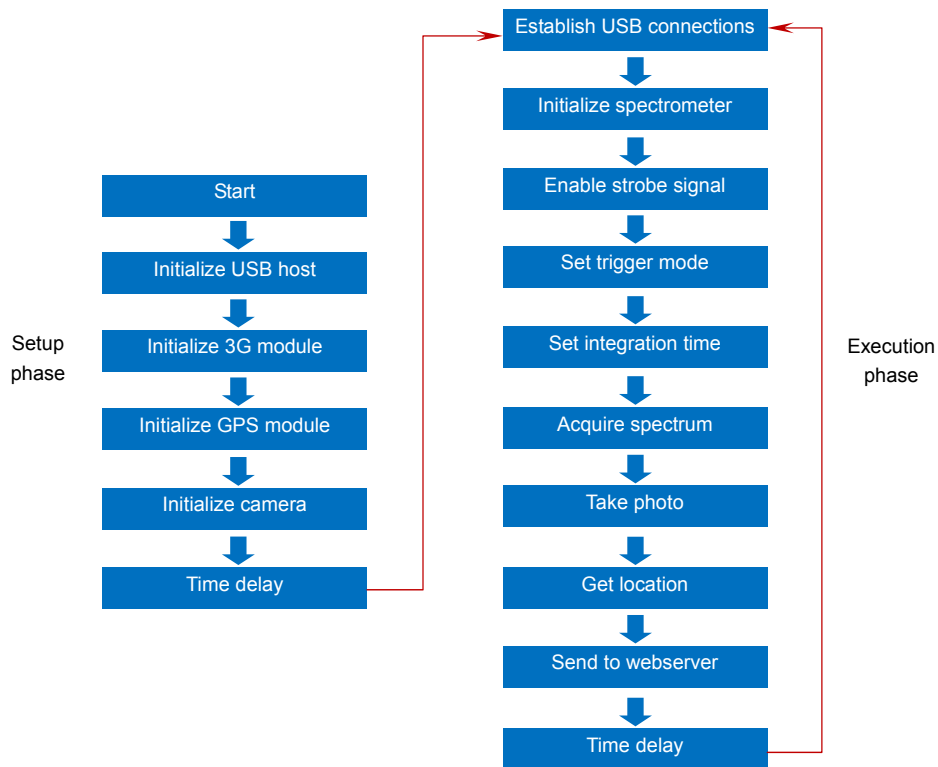
Fig. 3　Data acquisition flow.

per month. EC2 adopted in the optical system enables quicker access of spectra data in real time. Amazon provides a huge range of web services and in this project the Virtual Service in the Cloud, Elastic Compute Cloud (EC2), was adopted. A free tier Ubuntu Server 14.04 LTS (PV), SSD Volume Type, was selected under EC2 instance.

2.2　Data acquisition flow

The data flow of the system is illustrated in Fig. 3, which mainly consists of two parts: (i) setup phase, and (ii) execution phase. In the setup phase, the USB650 spectrometer has to be initialized each time when a spectrum is taken, and the 4096 bytes of data collected need to be converted into 2048 spectra data before follow-up processing. In the execution phase, the functions of spectra acquisition, image capture, location tracking and wireless transmission will be achieved in sequence.

3　Results and discussion

The final prototype of the portable optical sensing system is illustrated in Fig. 4, and an experiment was conducted to demonstrate the effectiveness of the prototype.

In the experiment, three water samples were analyzed, firstly tea water, secondly sea water from West Coast Park of Singapore, and thirdly laboratory tap water, as shown in Fig. 5(a). A laser source with central wavelength at 532 nm, power 300 mW was used with the spectrometer integration time of 2 s. The experimental results based on the data downloaded from our cloud database after 50

points smoothing are shown in Fig. 5(b). It is concluded that the tea water emits the strongest fluorescence, followed by sea water, while laboratory tap water has no fluorescence emitted. The spectra peak intensity at 548 nm of sea water may result from the existence of some microbes. The peaks at 650 nm are present for both sea and laboratory tap water samples, which might be attributed to the presence of stray light. The GPS coordinates have been accurately obtained by our system (1.299N, 103.772E) which is the exact position of our laboratory. This is only an application demonstration experiment, and the system is not limited to water testing. It is also suitable for paper testing as well as many applications in the biochemistry field.
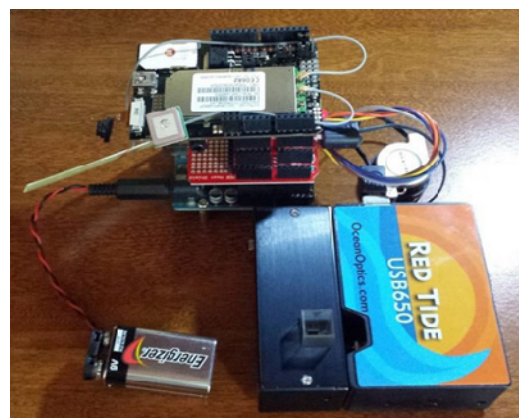

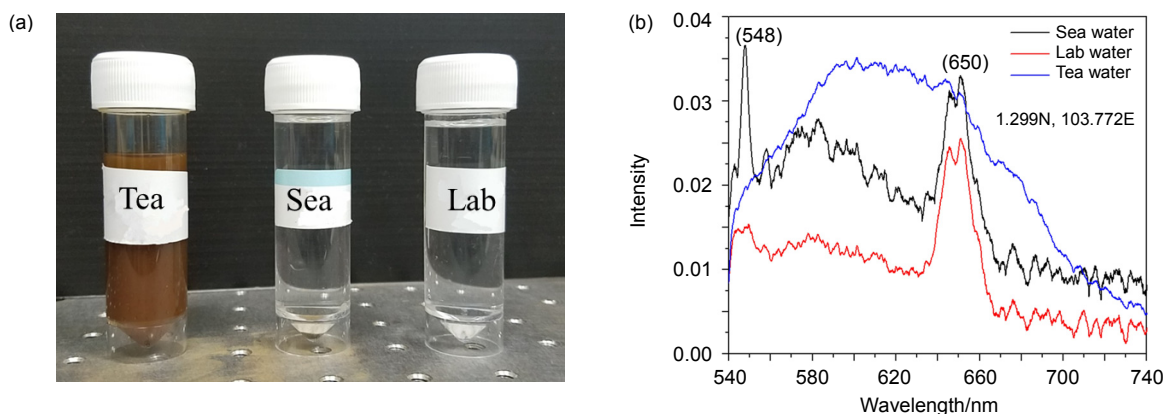Fig. 4　Prototype of the portable optical sensing system.

Fig. 5   Testing samples and the experimental results. (a) Three water samples for testing. (b) Fluorescence spectra of the three water samples.

4   Conclusions

The details regarding the fundamental of a portable optical sensing system to rapidly obtain the fluorescence spectra of samples is presented in this paper. A compact configuration is achieved by integrating a small spectrometer as an optical sensor, a microcontroller for issuing commands, a USB Host Shield for internal communication, a network module for external communication, and a web server for storing database and distributing results. A special software is programmed to extract the spectra from the spectrometer, capture images of the samples, acquire GPS location, and communicate with a cloud server. Since optical sensor and wireless communication module are adopted, the system can offer real-time detection capability. The fluorescence spectra of three water samples have been detected using our system within a short time, thus validating the system's effectiveness.

Acknowledgements

References

1   Albani J R. Principles and applications of fluorescence spectroscopy[M]. Oxford Ames, Iowa: John Wiley & Sons, 2007.

2   Guilbault G G. Practical fluorescence[M]. New York: CRC Press, 1990.

3   Eaton-Magaña S, Post J E, Heaney P J, et al. Fluorescence spectra of colored diamonds using a rapid, mobile spectrometer [J]. Gems & Gemology, 2007, **43**(4): 332–351.

4   Marsala A F, Loermans T, Shen S, et al. Portable energy-dispersive X-ray fluorescence integrates mineralogy and chemostratigraphy into real-time formation evaluation[J]. Petrophysics, 2012, **53**(2): 102–109.

5   Yukawa H, Baba Y. In vivo fluorescence imaging and the diagnosis of stem cells using quantum dots for regenerative medicine[J]. Analytical Chemistry, 2017, **89**(5): 2671–2681.

6   Elgemeie G H, Ahmed K A, Ahmed E A, et al. A simple approach for the synthesis of coumarin fluorescent dyes under microwave irradiation and their application in textile printing[J]. Pigment & Resin Technology, 2016, **45**(4): 217–224.

7   Lenhardt L, Bro R, Zeković I, et al. Fluorescence spectroscopy coupled with PARAFAC and PLS DA for characterization and classification of honey[J]. Food Chemistry, 2015, **175**: 284–291.

8   Karoui R, Blecker C. Fluorescence spectroscopy measurement for quality assessment of food systems-a review[J]. Food and Bioprocess Technology, 2011, **4**(3): 364–386.

9   Huang C J, Dostalek J, Sessitsch A, et al. Long-range surface plasmon-enhanced fluorescence spectroscopy biosensor for ultrasensitive detection of E. coli O157: H7[J]. Analytical Chemistry, 2011, **83**(3): 674–677.

10   Yang Jian, Shi Shuo, Gong Wei, et al. The characterization of plant species using first-derivative fluorescence spectra[J]. Luminescence, 2017, **32**(3): 348–352.

11   Lin L, Dikeman R, Molini B, et al. Photochemical treatment of platelet concentrates with amotosalen and long-wavelength ultraviolet light inactivates a broad spectrum of pathogenic bacteria[J]. Transfusion, 2004, **44**(10): 1496–1504.

12   Wachsmuth M, Conrad C, Bulkescher J, et al. High-throughput fluorescence correlation spectroscopy enables analysis of proteome dynamics in living cells[J]. Nature Biotechnology, 2015, **33**(4): 384–389.

13   Butte P, Lapchak P, Kittle D S. Time-resolved laser-induced fluorescence spectroscopy systems and uses thereof: U.S. Patent, 20160377547[P]. 2016-12-29.

14   USB-650 red tide spectrometers[EB/OL]. https://oceanoptics. com/product/usb-650-red-tide-spectrometers/.

15   Arduino & Genuino UNO[EB/OL]. https://www.arduino.cc/en/ Main/ ArduinoBoardUno/.