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Developing a mobile app for remote access to and data analysis of spectra

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ABSTRACT

Vibrational spectroscopy is a non-destructive analytical method that can be used to analyse a wide range of materials. A vibrational spectrum contains information on the chemical structure of the sample being analysed, which can be recorded rapidly. With hand held mobile device technology being considered as a relatively mature market, there is an excellent opportunity to combine vibrational spectroscopy with mobile devices for in situ analysis of samples. There are still instances where analytical instruments require being linked to desktop PC's/laptops for instrument control and data manipulation. However, mobile devices are becoming increasingly more powerful thus, enabling data manipulation on devices via cloud based technology. With desktop PC's and laptops often having a larger environment footprint than the instrumental spectrometer itself, this therefore highlights the potential for mobile spectroscopy devices. This paper reports the first development of an app (SpectralAnalyser) to enable the use of mobile devices to access and manipulate spectra and describes the different approaches and implementation issues considered during the development of apps to display spectra on Android and iOS platforms.

1. Introduction

Vibrational spectroscopy, such as Raman and Infrared (IR) spectroscopy are proven analytical methods, which have been used to analyse a wide range of materials. With only simple sample preparation required, a spectrum, which contains information on the chemical composition of the material being analysed, can be recorded rapidly. As well as this, the instrumentation needed to record a vibrational spectrum is simple to operate and relatively cheap i.e. no expensive reagents needed. Because of these advantages, vibrational spectroscopy has been applied to many real world problems in many varied areas, such as biomedical [1,2], defence [3,4], forensics [5], astrochemistry [6], for bio-signatures in the martian environment [7].

For instance, in the biomedical sphere, vibrational spectroscopy has been shown to be a valued technique in the analysis of serum [8], capable of discriminating high grade brain tumours, low-grade brain tumours and normal patients from 1 μl of human serum to sensitivities and specificities of 93.8 and 96.5% respectively [9], classifying ovarian cancer to an accuracy of 96.7% using plasma samples [10]. Raman spectroscopy has recently been shown to be capable of discriminating metastatic brain cancer, high grade brain cancer and normal cancer from tissue samples using a small wavenumber range of 600–800 cm^{-1} to a sensitivity and specificity of 100% and 94.44% for high grade cancer, 96.55% and 100% for metastatic brain and 85.71% and 100% for normal brain tissue spectra [11]. In addition, FTIR has proven to be an excellent analytical technique to quickly determine heavy water concentration in pressurised heavy water reactor [12] and FTIR and Raman are capable of remote sensing of Chemical Warfare Agents (CWAs) [13].

A relatively mature market in hand held instruments and configurable technology provide an excellent opportunity for enabling mobile in situ analysis of samples using vibrational spectroscopy, however in situations as described above an ability to place the spectrometer in a different location to the feedback system would be of great advantage. For instance, a miniature spectrometer with cloud based data feedback could be placed in a hazardous location to monitor air quality thus, providing real time results back to scientists outside the hazardous area, or a spectrometer could be placed in a clinical theatre without the need for an operator inside therefore, minimising the risk of infection. Currently this is not possible.

Developments in the mobile/miniature spectrometer technology and in situ use of spectroscopy require appropriate

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coinciding developments in software and applications. Some mobile/miniature spectrometers require the spectrometer to be linked to a desktop PC/laptop for instrument control and data acquisition. However, often the desktop PC/laptop has a greater environmental footprint than the spectrometer instrument.

A mobile applet (app) capable of accessing/manipulating data would prove extremely useful and the applications wide and varied. In this study we describe the development of apps for the interrogation and manipulation of vibrational spectra using Android and iOS platforms with cloud-based technology and investigate the different development approaches required and the implementation issues arising with each platform.

2. Methods and tools

2.1. Development approach

Small prototype apps were developed to evaluate the graphics and user interface libraries. Once the libraries had been selected, an iterative incremental approach was used. Requirements for each iteration, a fixed period or "timebox" of two weeks, were defined and prioritised before each iteration as MoSCoW lists based on client feedback. MoSCoW is a "prioritisation technique used in business analysis and software development to reach a common understanding with stakeholders on the importance they place on the delivery of each requirement" [14]. The client classifies the tasks for an iteration as "Must have", "Should have" "Could have", "Would like, but won't be implemented". The developer indicates the expected time each task should take. To be used effectively, timeboxing requires at most 60% of the requirements to be of type "Must have", so the client and developer can be confident that they will be achieved within the timebox.

The iterative lifecycle ensured testing was continuous. A benefit of the Android platform is the heterogeneity of its target devices. However, this still requires rigorous device testing to ensure a consistent user experience. During development, the application was tested primarily on a HTC One X handset, and also on a Nexus 7 tablet and a Kindle Fire tablet. The Android Device Emulator was used during development. However, user interface testing on the emulator is limited as touch screen gestures cannot be truly simulated using a mouse. The iOS app was tested on an iPhone and an iPad as well as the iOS emulator.

2.2. A cross-platform application using Qt

Qt is a cross-platform development framework based on C++ [15]. An initial prototype was written using Necessitas 4.8.2, a version of Qt which aims to support Android implementations [16] and the QCustomPlot graphics library [17]. However, although the implementation ran on an Android-based Nexus 7 tablet, it was not possible to implement the gesture-based interaction expected of a mobile application and development switched to O.S.-specific environments.

2.3. Android application

2.3.1. Development environment and graphics library

The development used the Eclipse IDE, which is the most common environment for the Android Software Development Kit (SDK) [18] and provides facilities for writing, testing and debugging Android applications, this includes integration with the Android emulator and Android devices. Android applications use the Java programming language, compiled for the Dalvik virtual machine.

Several graphics libraries, GraphView [19], AFreeChart [20], and AChartEngine [21] were evaluated through prototypes. The demonstration using GraphView was sluggish on a Nexus 7 tablet, but both AFreeChart and AChartEngine provided appropriate facilities and performed adequately on the Nexus 7, a Kindle Fire, and an Android phone.

2.3.2. User interface

The Android application uses an Action bar across the top of the screen. Since commonly used actions such as "Load" and "Subtract" are always visible, the user can quickly control the application. However, because of the Action bar, the application is only supported on devices that have Android 3.0 and above. Less common actions such as logging into Dropbox or peak selection are accessed through the "action overflow" button of the Action bar, so not to overwhelm the user.

Touch, pinch and pan gestures allow the user to select and manipulate spectra. However, when labelling peaks, the user must use the zoom toolbar to vary the number of annotations displayed.

2.3.3. Program structure

The Android application framework is based around "Activities", "a single focused thing that the user can do" [22]. The code within an Activity is initially executed through callback methods activated at appropriate stages of the Activity Lifecycle, e.g. when the activity is created, started, paused, resumed or destroyed.

The application has a single activity, which creates the action bar buttons and the view of the graph and attaches appropriate event handlers to respond to input events.

Interaction with Dropbox (see Section 2.5.1) uses an `AsyncTask` object, allowing the user interface thread to initiate and display the results of a background operation, while maintaining responsiveness to the user while the background task is running. The developer provides a `doInBackGround` method that is executed by a background thread and a `doPostExecute` method that is executed on the user interface thread after the background task has completed.

2.4. iOS application

2.4.1. Development environment and graphics library

The program was written in Objective C using the XCode IDE, which provides facilities for writing, testing and debugging iOS applications, including integration with the iOS emulator and IPhone/IPad devices. The key algorithms for processing spectra were translated from Java. The Core-plot graphics library [23] provided the necessary facilities and appropriate performance.

2.4.2. User interface

An Action bar approach was emulated using icons, most of which have two actions depending on whether they are pressed or held down, this saves screen space and simplifies the interface. Whereas menus in the Android application appear in a Dialog box, the iOS application has a separate view, implemented by ECSlidingViewController [24] which slides in from the left. This view is populated either with the available Cloud and local files or with the spectra that can be selected (e.g. to annotate peaks).

The iOS application also allows pinch and pan gestures. However, it does not require an extra toolbar to increase the number of annotations. Instead, it automatically decides which peaks to label depending on the zoom level.

2.4.3. Program structure

Asynchronous interaction with Dropbox (see Section 2.5.1) that allows the user interface to remain responsive is provided automatically by the DropBox iOS API. Methods such as `[DBRestClient loadFile:intoPath:]` are asynchronous and return immediately rather than when the requested action is completed. The developer implements event handers for

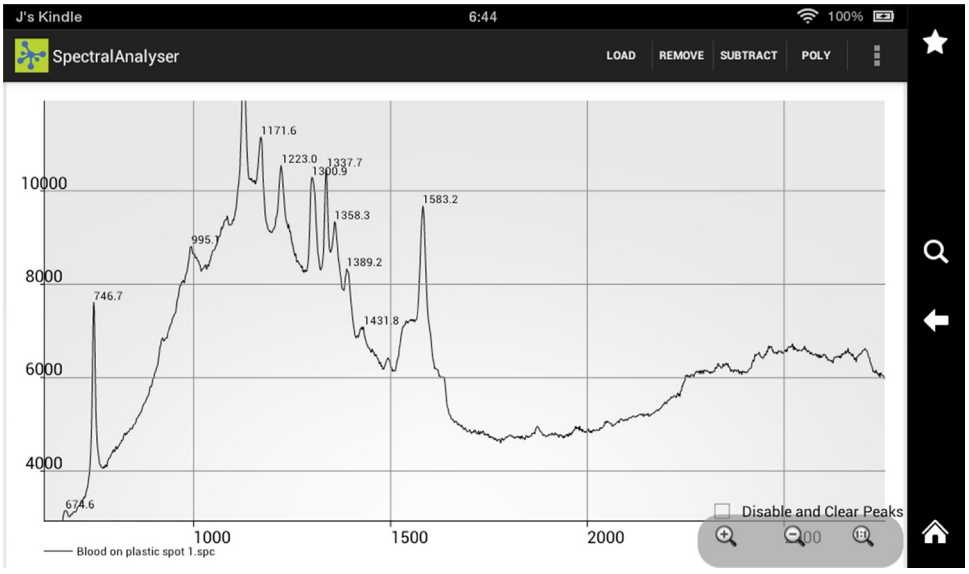

Fig. 1. Android App displaying a spectrum with labelled peaks.

`[DBRestClient loadedFile: contentType: metadata:]` and `[DBRestClient loadFileFailedWithError:.`

One of these is called when the action is completed and displays the results to the user.

2.5. Data storage

2.5.1. Accessing DropBox

The Dropbox API for Android or iOS devices [25,26] is a RESTful API that uses the OAuth protocol to allow an application to access a folder in the user's Dropbox area across the Web. To use the API, a developer must create an online Dropbox application linked to the developer's Dropbox account. This generates an "app key" and "secret key" used to authenticate the application when Dropbox seeks authorisation from the user to allow the application to access the user's area. In development, a Dropbox application can be tested by up to five users. After the application has been approved by Dropbox, multiple users can use the service.

2.5.2. SPC file format

Spectrometers commonly output data in the binary SPC format [27]. The SPC format is complex as it can store *X*-*Y* measurements in a variety of different ways. For example, if the *X*-values are equally spaced, the data can be compressed by storing the initial *X*-value, the increment between *X*-values and all the *Y*-values. The precise structure of the data in an SPC format file is defined in a header block: based on the information this contains, the application can interpret the data stored in the rest of the file.

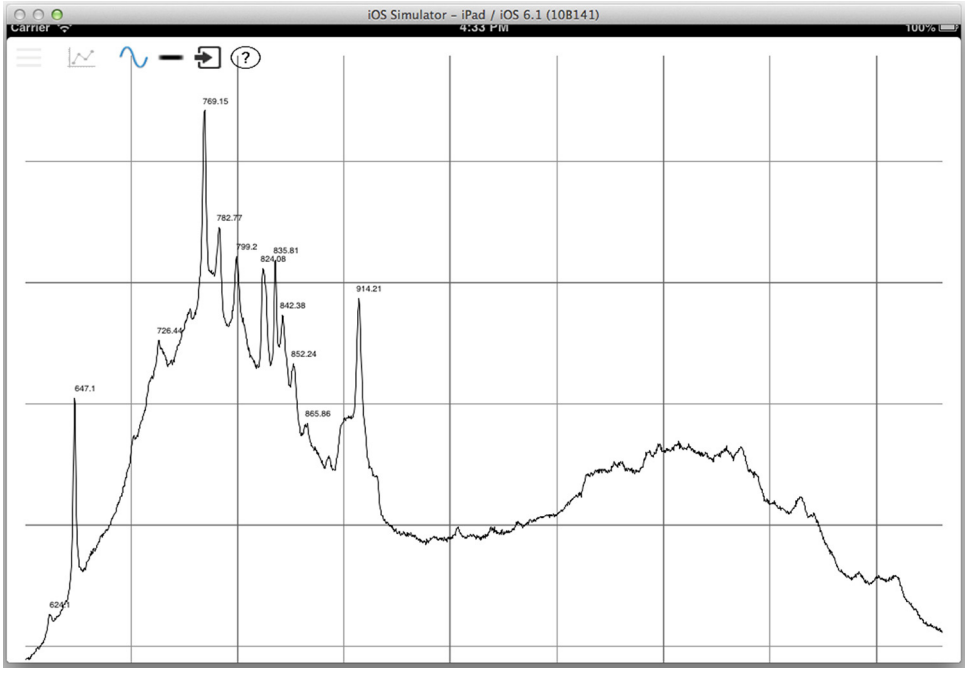

Fig. 2. iOS App displaying a spectrum with labelled peaks.

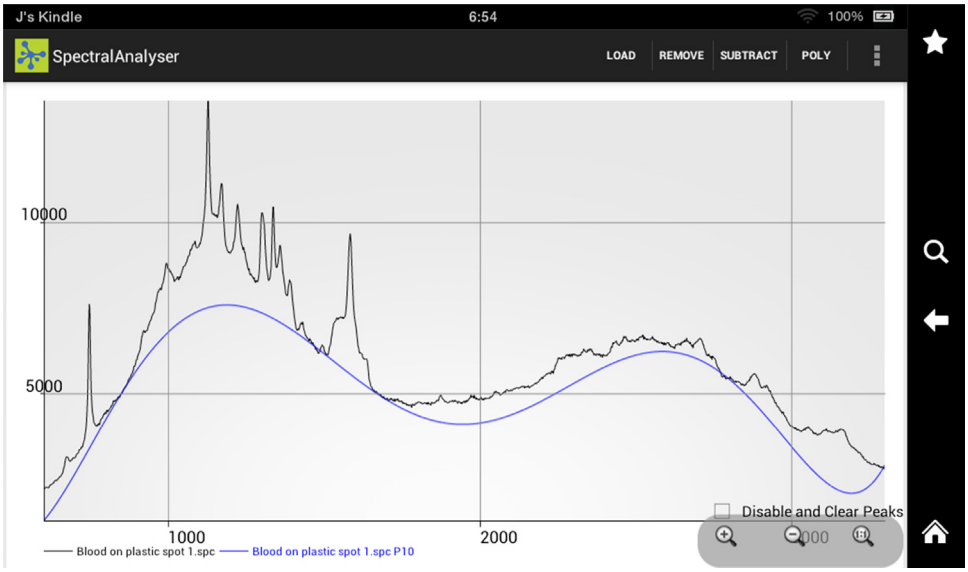

Fig. 3. Android App displaying a spectrum and an order 6 polynomial approximation.

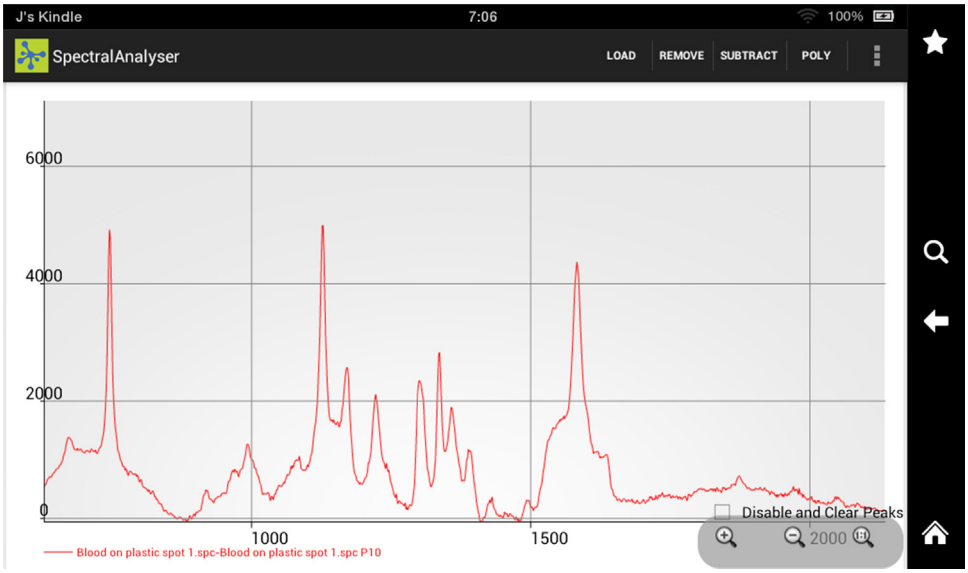

Fig. 4. Android App displaying a spectrum after subtraction of an order 6 polynomial approximation.

3. Results

Information about the Apps is available at http://www.note-ed.org/sp/, where the Apps will be made available for download.

3.1. Facilities

3.1.1. Sources of data

The user can retrieve spectra from both local and Dropbox storage and parse and display text files containing tab-separated data or binary files in common SPC formats (evenly spaced *X*-values and unevenly spaced *X* values).

3.1.2. Data manipulation

Multiple spectra can be displayed and manipulated using pinch gestures for zoom and flicking or drag gestures to pan.

Spectra loaded from storage or generated by the polynomial approximation tool can be subtracted from each other (see Figs. 2 and 3). At this present time no scaling is possible.

3.1.3. Peak detection and annotation

A simple peak detection algorithm was implemented to identify a *y*-value that is greater than its neighbours on either side of a peak. To reduce the risk of spurious peak detection, a neighbourhood of 26 values is used by default and the peak also has to be greater than 5% above the average of those values. Depending on the level of zoom, the number of annotations will increase or decrease (Figs. 1 and 2).

3.1.4. Simple noise processing

As explained by Kourkoumelis et al. [28] the interpretation of Raman spectra is often hindered by a broad background signal, which is mostly due to fluorescence from organic molecules and

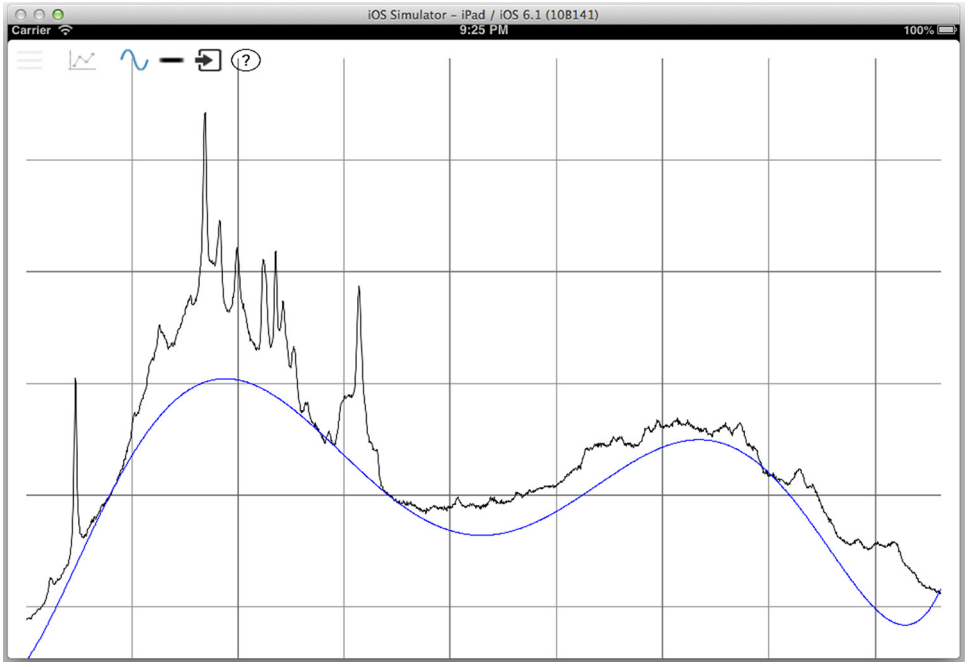

Fig. 5. iOS App displaying a spectrum and an order 6 polynomial approximation.

contaminants. To try to remove fluorescent background noise, a low-order polynomial approximation of the spectrum can be subtracted from the original (Figs. 3–6). Two algorithms were explored: least squares approximation and Chebyshev approximation [29]. The least squares approximation minimises the average error in the approximation whereas the Chebyshev approximation minimises the maximum error and reduces the risk of significant localised error. Both performed well for polynomials up to order 5, but as it avoids the potentially ill-conditioned numerical matrix inversion used for least squares approximation, the use of the orthogonal Chebyshev polynomials [30] means that any order of approximation can be robustly computed.

3.2. Evaluation

3.2.1. Development environment and programming language

The XCode and Eclipse environments provide similar facilities for the programmer (code completion, debugging facilities, including the ability to debug on an attached device, and an emulator). The fact that Eclipse can be used on Windows and Linux OS, whereas XCode only runs on MacOS, means that Android development is slightly more portable.

Although the message syntax of Objective C is unusual for programmers familiar with C++ or Java, there is no difference in the power of the languages used.

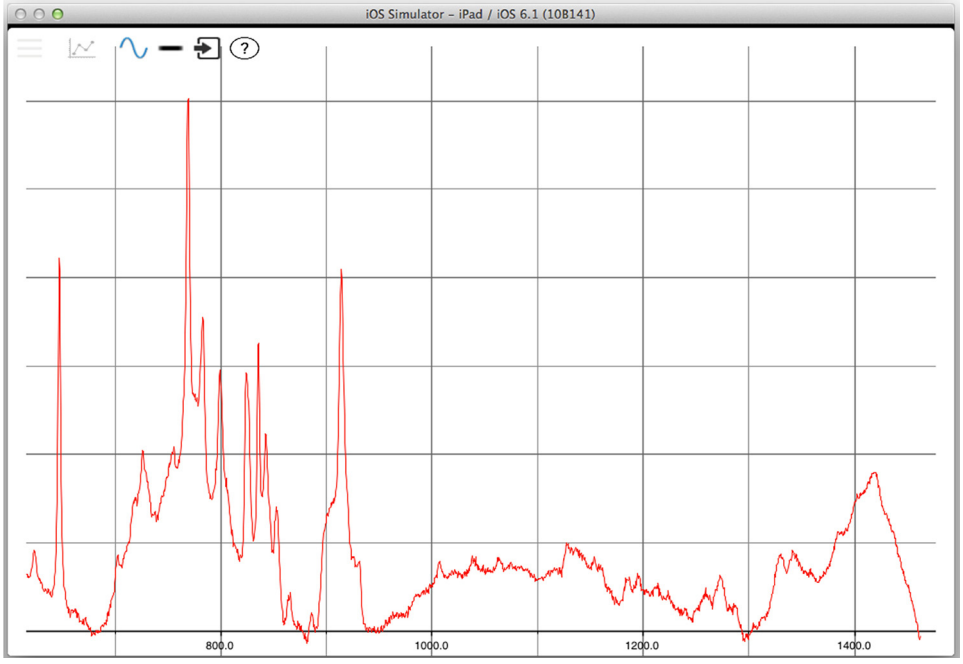

Fig. 6. iOS App displaying a spectrum after subtraction of an order 6 polynomial approximation.

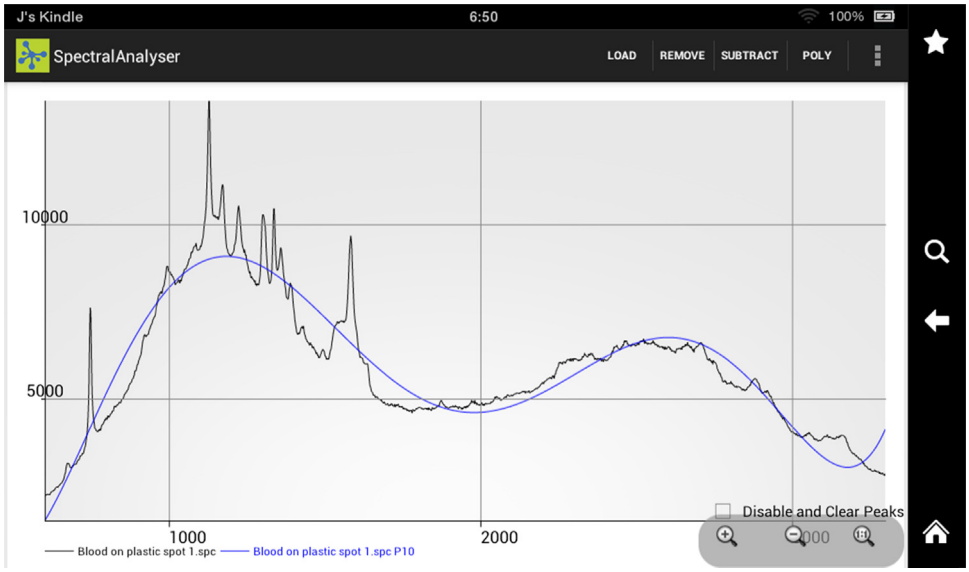

Fig. 7. Android App displaying a spectrum and an order 6 polynomial approximation.

An Android app can be freely deployed simply by making the executable (.apk) file available to testers by email or through a Web site. Deployment through Google Play requires some additional administrative steps. However, to reduce the risk of malicious apps, the deployment of iOS apps is considerably more onerous. Even for testing, a certificate has to be generated for each target device.

3.2.2. Usability

The two graphics libraries, AChartEngine for Android and Core-plot for iOS, provided appropriate facilities for these apps and performed adequately when displaying files with several thousand points. Both Android and iOS apps reacted responsively to drag and pinch interactions.

The user interfaces on both apps allow the user to access all the facilities simply. However, separate menus were used to select spectra in the iOS application. It is more natural to choose a drawn spectrum by touching it rather than selecting it from a menu. Where two spectra are too close to be selected by touch, selecting the displayed title provides a natural alternative without requiring additional screen space or a pop-up/slide-in menu.

3.2.3. Elimination of background fluorescence

Because the polynomial curve originally fitted to the whole spectrum included regions with significant Raman peaks and regions with only background fluorescence, it overestimated the background signal (see Figs. 7 and 8). An improved estimate can be obtained by fitting the curve to regions that the user selects as not containing significant Raman peaks or by applying an automated algorithm (e.g. Modified Polyfit [31], I-ModPoly [32]) designed to ignore significant peaks. Since user selection can be slow and

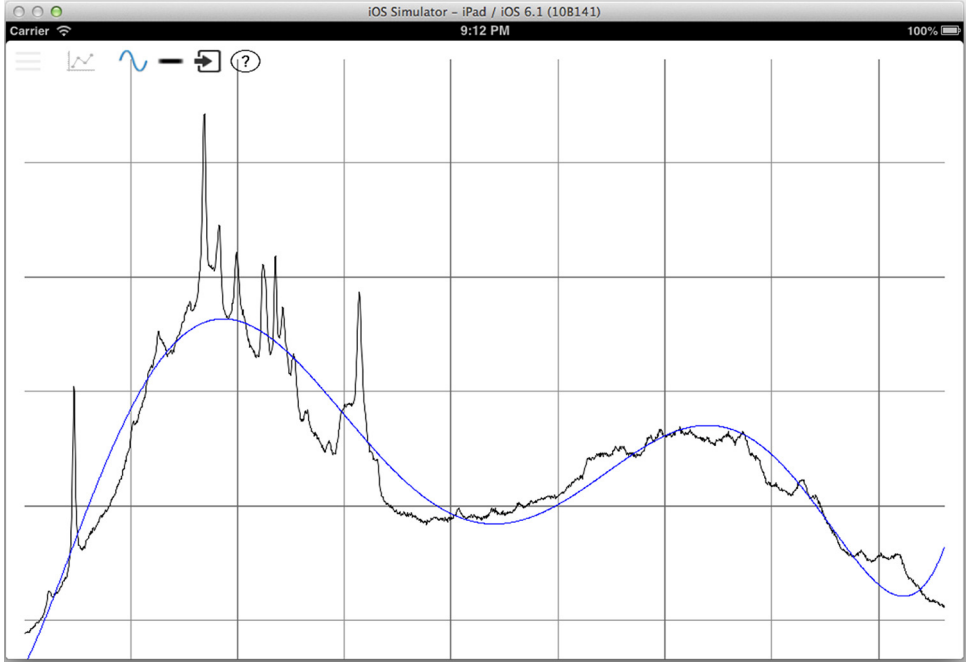

Fig. 8. iOS App displaying a spectrum and an order 6 polynomial approximation.

difficult even when using a mouse and will be particularly difficult using a touch screen, an automated algorithm is preferable. A simple variant of the Polyfit algorithm was implemented. After fitting an initial polynomial to the spectral data, the spectral values above the polynomial were replaced by the value of the polynomial approximation. This process was repeated 50 times (compare Figs. 3 and 5 with Figs. 7 and 8). The effectiveness and efficiency of more complex automated algorithms will be evaluated.

4. Conclusion

The use of mobile apps for data manipulation enables vibrational spectroscopy to reach its potential for in situ analysis. Through releasing the requirement for a desktop PC/laptop for data analysis, there could potentially be more scope for the application of vibrational spectroscopy in clinical and potentially dangerous industrial environments. Not to mention the greater flexibility a mobile app would bring to data analysis. The ease of use of a mobile app would mean that typical spectral analysis, or even live spectral monitoring tasks could be performed from home or while on public transport, without the need for environmentally expensive PC's.

The process of creating these applications has proven that the mobile analysis of spectra is possible and that cloud storage is a viable way to transmit data to a device. Because Dropbox has a freely available software development kit, it was used as the cloud storage provider for this application. However, an alternative web service could be used, but would require software changes.

Future work will include:

- Improving the usability of both applications following feedback, and increasing the range of Android handsets supported.
- Providing additional data manipulation features e.g. median filtering to remove shot error.
- Creating an online web service to provide cloud storage instead of using Dropbox. As well as providing greater flexibility, this will allow more computationally intensive server-side analysis of spectra, such as pattern analysis and a peak identification service.

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