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Smartphone-based Chemistry Instrumentation: Digitization of Colorimetric Measurements

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This report presents a mobile instrumentation platform based on a smartphone using its built-in functions for colorimetric diagnosis. The color change as a result of detection is taken as a picture through a CCD camera built in the smartphone, and is evaluated in the form of the hue value to give the well-defined relationship between the color and the concentration. To prove the concept in the present work, proton concentration measurements were conducted on pH paper coupled with a smartphone for demonstration. This report is believed to show the possibility of adapting a smartphone to a mobile analytical transducer, and more applications for bioanalysis are expected to be developed using other built-in functions of the smartphone.

Key Words : Colorimetric measurement, Smartphone, Snapshot technique, Mobile instrument, pH measurement

Introduction

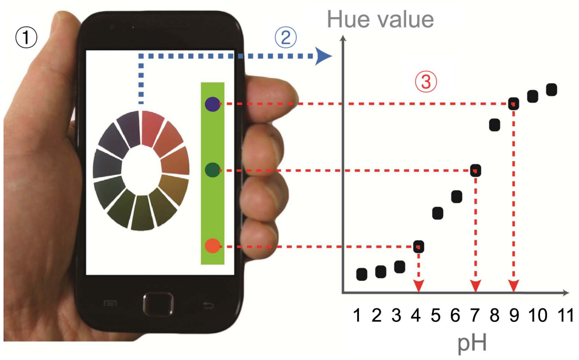
Being inspired by the question, “mobile computing platforms such as the iPhone are beginning to make inroads into the laboratory-serious prospect or fairy tale?”,[1] and pursuing easy handheld detector for diagnostics,[2] here I report an interesting technique that a smartphone is used as a mobile diagnostic transducer. Smartphones such as iPhones and android phones are integrated devices of the cutting edge technologies such as fast CPUs, user-friendly interfaces, high quality digital cameras, GPS, gyro sensors and so on. Besides, it is supplied with software development toolkits for controlling the hardware,[3] to provide a flexible development platform. As a result, a huge number of mobile phone apps have been made as shown in the app market, and sometimes they come with auxiliary devices attached to the smartphones.[3(c)] In this article, such a smartphone is utilized as a signal transducer replacing a spectrometer, and a mobile instrumentation platform for analytical applications so-called “lab-on-a-smartphone” will be suggested for development of portable measurement devices.

A colorimetric method is well-known, and attractive because it provides easy, cheap, and on-site diagnostic means. The best benefit from this method is that the signal even can be detected by the naked eyes. Owing to that, no auxiliary electronic device is needed for detection. On the other side of this benefit is the weak point that the visual determination has poor accuracy and depends on environmental and personal conditions. Even though suitable detectors have been proposed,[4] there have still been needs for simple and easy detection tools.[2] In this report, a smartphone takes over the role of that, which means we do not have to buy additional detecting spectrometer if we are already smartphone users.

To prove the concept of using a smartphone as a colorimetric detector, here I conducted pH paper tests. As one of the classic, fundamental colorimetric methods, pH paper measures the concentration of protons in solution, and represents the results as colors recognized by eyes. Due to cheap and easy handling of it, the pH paper test is still frequently used while the pH meter with an expensive glass membrane electrode is used for precise measurement. However, as mentioned above, such naked eye detection is not appropriate for precise measurement. Especially, when the measured color is positioned between reference pH colors, appropriate estimation of pH is hardly made. In this article, inheriting the advantage and overcoming the week point in using the paper-based colorimetry, a smartphone is used to digitize the observed color to physical or chemical values: the smartphone takes a picture of pH paper with the reference colors.

Theoretical Consideration. The principle of pH paper measurement is that the indicating chemicals change their colors according to the concentration of protons. In many types of pH paper, the colors for indication are red, green, and blue from low to high pHs.[5] Coincidently, the order of these colors matches that of visible light spectrum from long to short wavelengths. Hence, the colors of the pH paper can be correlated to the light spectrum, and determination of pH by color change can be quantitatively made with a spectrometer. However, use of the spectrometer does not suit to the purpose of pH paper usage because it costs much, maybe more than a digital pH electrode, and is bulky and not handheld. Even though a spectrometer is the best device that can accurately measure the color, it can be replaced by simpler electronic optical devices only if they can distinguish colors like a CCD camera. A smartphone is one of the best candidates because it contains an optical sensor, and can analyze the signal by itself due to its mobile computing power. All the processes can be programmable and conducted based on the user-friendly interface for easy and point-of-care use.[6]

Scheme 1 depicts the technical processes. The first step is to take a picture of reference colors with samples, the second



Scheme 1. Processes of the smartphone-based colorimetric measurement.

step is to make a calibration curve from the reference colors, and the third step is to find the color positions of the samples on the calibrated curve.

However, here are two problems encountered at the transition from the first to the second steps. One is that the colors taken in the picture are digitized on the RGB color coordinate,[7] hence calibration is not easily made because the RGB color space is not directly related to the wavelengths of the light spectrum. The other problem is that the digital camera has optical sensors with filters of red, green, and blue, and the detected colors have only limited wavelengths, consequently. In order to solve these problems, hue values of the colors are used as the variable instead of the wavelength. A color plotted on the RGB color space can also be transferred to the HSV color space without changing the original color.[7,8] The HSV space has three variables for expressing a color, which are hue (H), saturation (S), and brightness (V) instead of R, G, and B. Even though H, S, and V are needed to fully express a color, only H is needed to discriminate the colors of specific frequencies because H represents the primary colors or combinations of them and distinguishes one color family from another.[8] And S and V contain other supplementary information on the color details. Since the colorimetry measures only the types of color (not the spectrum intensities of wavelengths), H values extracted from RGB pixels are used to correlate the color on pH paper to pH values. The H value can be calculated through known algorithms with appropriate equations,[7] and also be obtained easily in Matlab using the RGB2HSV function.[9]

Experimental

Materials. Sodium citrate, citric acid, KH_2PO_4, K_2HPO_4, NaH_2PO_4, Na_2HPO_4, boric acid, and NaOH were purchased from Aldrich. Appropriate amounts of these chemicals were dissolved in doubly deionized water to prepare buffer solutions of pH 4.0, 7.0, 7.4, and 9.0 according to the procedures in the reference.[10] A roll of pH paper strip was purchased from Advantec (Toyo Kaisha, Japan). The smartphone used for taking pictures is Galaxy from Samsung electronics (Korea).

Procedure. The colors of the reference pH and samples on pH paper were taken in a single snapshot through the built-in CCD camera of the smartphone with various white balance options. Once the images were transferred to a PC, they were analyzed on Matlab. The color coordinate of a pixel was transformed from RGB to HSV using the RGB2HSV function supplied by Matlab.[9] Then, only H values were extracted, and averaged within the same color area.

Results and Discussion

Figure 1 shows the actual picture of the reference colors of pH taken by the smartphone, and the calibration curve. In (a), H values were obtained along the dotted line around the wheel, and the values in each color were averaged to be assigned to the color's pH. By plotting the H values along the pH, we obtained a calibration curve in (b). Even though the relationship is not linear, reliable quantification can be achieved through careful calibration as will be described below.

In order to confirm the relationship between the digitized color values and pHs, standard buffer solutions were tested on a pH paper strip: pH 4.0, 7.0, 9.0 and 7.4. The H values are plotted in Figure 2(a), and the averaged values of the first three samples are 0.11(± 0.0028), 0.24(± 0.0064), and 0.54(± 0.023), which correspond to pH 4.0, 7.0, and 8.9, respectively. Not only the pH values on the reference color

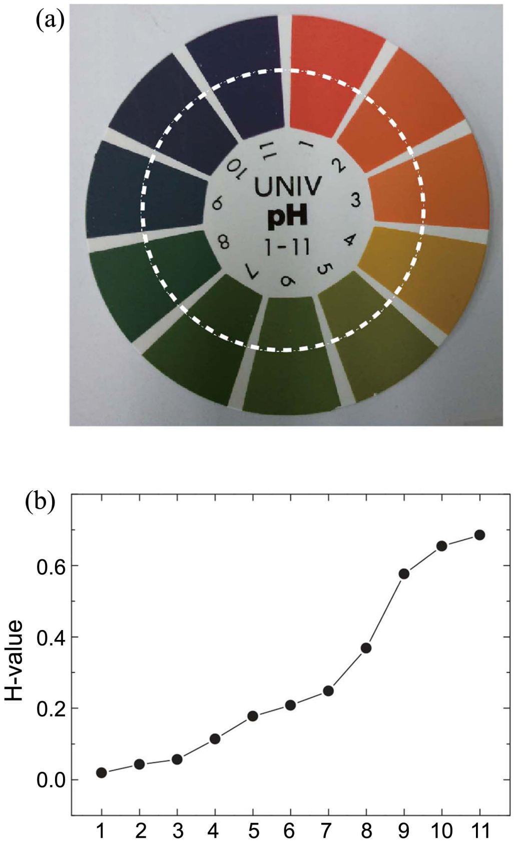


Figure 1. (a) The reference pH colors are taken in a picture using a smartphone, and (b) the reference colors around the white dotted line are digitized as H-values, and they are plotted along the pH.

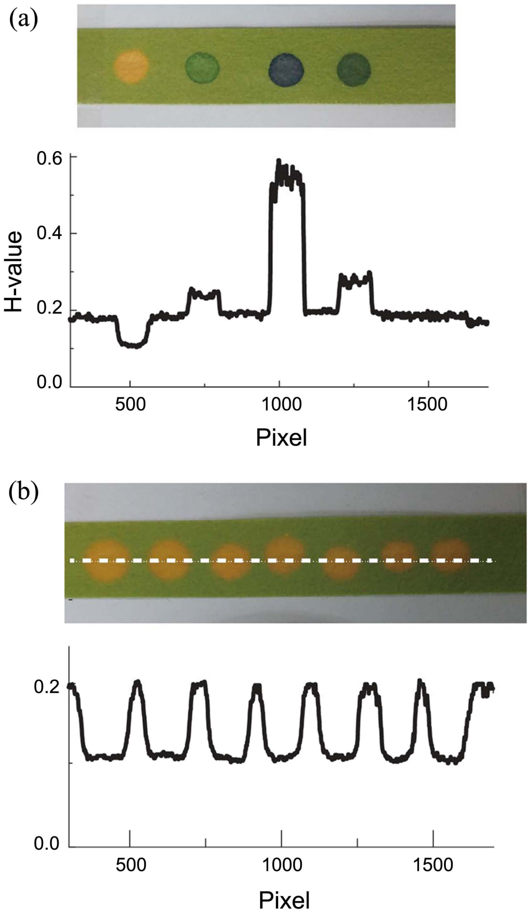


Figure 2. (a) Drops of different pH buffer solutions are tested on a single strip of pH paper to demonstrate the pH measurement. (b) Drops of pH 4.0 buffer solution are tested to confirm the reproducibility and reliability.

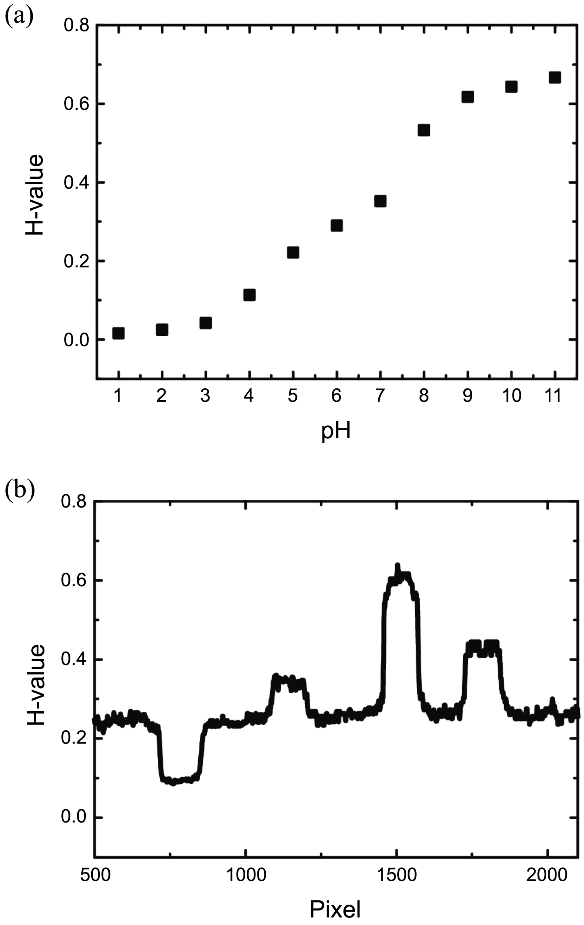


Figure 3. A pH measurement with an enhanced resolution was achieved by taking the picture with controlling the white balance. (a) the new calibration curve, and (b) digitized H-values of pH 4.0, 7.0, 9.0, and 7.4.

wheel, but a pH value between two reference pH colors was measured. Assuming that the pH and the digitized color value are linear within the range between two reference colors, we estimated the pH value of the color, of which the H value is placed between two reference values. Here we tested pH 7.4 solution, and its digitized value was 0.275 (± 0.0077) corresponding to pH 7.3. As a result, we were convinced of that the digitized pH values from the measured colors correctly match the pH of the actual solutions. Also, reproducible quantification was examined. The colors of pH 4.0 solutions are sampled, and were digitized and plotted in Figure 2(b). The result represents reliable reproducibility of the digitization. The reproducibility was also confirmed using a smartphone-based tablet, iPad of Apple computer.

As color is sensitive to light, digitization of colors depends on light, and gives different outputs depending on the white balance.[7] Taking advantage of that, the dynamic range of colorimetric measurement is easily controlled by adjusting the white balance of the picture. In Figure 2(a), the H value of pH 7.4 was obtained close to that of pH 7.0 because the range of the H value between pH 7 and 8 is narrow. To improve the resolution of the H value of that specific region, the white balance was controlled to widen the range of the H values specifically. Figure 3(a) is the new calibration curve obtained with the appropriate white balance, which widens the range of the H value between pH 7 and 8 from 0.12 to 0.18. As a result, the improved signal of pH 7.4 was obtained, more distinguished from that of pH 7.0 as seen in Figure 3(b).

So far, we have described a technique of using a smartphone as a colorimetric digitizer. The significances of this work are viewed from two aspects. One is use of a smartphone for mobile instrumentation for chemical analysis using built-in functions of the smartphone, thus we can operate easy mobile measurements without complex and bulky devices. That implies that a smartphone provides a handheld mobile platform for laboratory works. The other aspect is that colorimetric measurement is carried out on a single snapshot picture. As all the information required is taken in a single picture, calibration and evaluation of multiple samples are managed simultaneously, which reduces time, labor, amounts of sample solutions, and inaccuracy.[11] And the results are obtained from types of colors rather than the intensity of colors, so that the background signal correction process is not necessary. Besides, control of the white balance allows us to change the dynamic range with an enhanced resolution for precise measurement over a specific range. Even though the computing processes in this report are performed by a desktop mathematics software, the mobile computing power of the smartphone will enable us to make an app capable of measuring and analyzing processes, and the app development is currently in progress in our laboratory. This method is also applicable to other colorimetric[12] and paper-based[13] diagnosis techniques for large scale arrays.[14]

Conclusion

In these days, smartphones become part of our lives, and platforms of traditional media such as books are changing to smartphones because they provide mobile multi-functions of high technology. Chemistry is in the same bandwagon.[6,15] While many applications being developed are related to information delivery based on smartphones such as electronic periodic tables and mobile paper reader apps, it has still been a question if they really make inroads into the laboratory. As this report demonstrated that chemical measurement was conducted based on a smartphone, we can say that the answer is very positive. Presumably, the first actual application will be connected to the colorimetric paper-based diagnosis. Even though the current work only uses the built-in camera for colorimetry, it is believed that other built-in functions of the smartphone sensing sound, temperature and magnetic field will be utilized for chemistry-related observations

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