An efficient and economical approach to hydrogen peroxide detection and neutralization utilizing molybdenum sensors

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Considering that significant challenges associated with the detection of peroxide-based explosives such as TATP and HMTD, as well as the fact that hydrogen peroxide (H_2O_2) is both a synthetic precursor and a degradation product of them, this study presents a rapid, cost-effective, and environmentally friendly approach for detecting and neutralizing H_2O_2 using Mo-based sensing devices. The method exploits the color change of a particular Mo compound, $Mo_2O_5(OH)$, from blue to pale yellow upon reaction with H_2O_2 , due to formation of MoO₃. For this work, butanol bronze-based test strips coated with Mo w

ere created and exposed to various concentrations of H_2O_2 . The color change was monitored using a camera and analyzed with ImageJ software. The reaction was found to follow a first-order kinetics, with the rate of color change proportional to the concentration of H_2O_2 . The slope of the phenomenological rate *versus* H_2O_2 concentration was found to be 16.752 color change % s⁻¹. The results demonstrate the high potential of Mo bronze-based test strips for low-cost detection and neutralization of H_2O_2 , offering a promising solution to the challenges posed by related dangerous explosives.

Keywords: Molybdenum, Hydrogen peroxide, Sensing devices

INTRODUCTION

The global rise in terrorist activities involving explosive devices has created an urgent need for effective methods to detect and neutralize these instruments [1]. Explosives, whether solid or liquid, exist in a metastable state, enabling rapid chemical reactions without external reactants such as oxygen. Peroxide-based explosives, particularly triacetone triperoxide (TATP) and hexamethylene triperoxide diamine (HMTD), have gained prominence due to their extensive use by terrorist organizations in the manufacturing of improvised explosive devices [13]. These cyclic peroxides pose a challenge for standard explosive detectors as they lack nitrogen-containing functional groups, making their identification [2]. Unfortunately, peroxide-based difficult explosives like TATP and HMTD continue to be used in numerous terrorist attacks, and attempts have been made to smuggle their precursor materials onto aircraft for in-flight bomb production [2, 3].

Hydrogen peroxide (H_2O_2) has found widespread industrial uses and applications and due to its property of being unstable and undergoing disproportionation, it is also used as a precursor for the synthesis of the aforementioned homemade explosives (TATP, HMTD), as well as several others and it is listed under peroxide-based energetic materials [4-9]. In view of this, it is generally accepted that H₂O₂ is a significant compound for determination of peroxide-based explosives [10-13]. As a result of the importance for improved detection methods that extend beyond traditional contexts and in particular the need for determining traces of H₂O₂, we present a rapid, cost-effective, and environmentally friendly approach for detecting and neutralizing it, using Mo sensing devices [14]. The choice of the Mo materials was due to selectivity, stability and intense color of its acompounds and the precedent of its applications in colorimetric detection of various species in solutions [10–13, 15]. Exploiting the reaction shown in equation (1), in which the original blue color of a Mo compound, Mo₂O₅(OH), with a metal charge transfer band at 710 nm, changes to a pale-yellow color (MoO₃) due to its reaction with H₂O₂, we designed Mo butanol bronze-based coated test strips and exposed them to various concentrations of H2O2

$$2\text{Mo}_2\text{O}_5(\text{OH}) + \text{H}_2\text{O}_2 \rightarrow 4\text{MoO}_3 + 2\text{H}_2\text{O}$$
(1)

The resulting color change was monitored using a camera to allow for the determination of the reaction kinetics and in particular how the rate of

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color change may be related to the concentration of H_2O_2 .

MATERIALS AND METHODS

All chemicals used in the experiment were of reagent grade (ACS reagent grade) and were employed without additional purification. UV spectrophotometric analysis was carried out using a Carey 50 UV-VIS spectrophotometer. Images of the test strips during exposure to H₂O₂ were captured using a Logitech Pro 9000 USB camera, and photographs were taken at 15 cm distance from the An open-source software (ImageJ), surface. provided by the National Institute of Health was used to perform image analysis to process the kinetic data. Butanol bronze was synthesized following the catalytic procedure outlined in the literature [16]. Test strips were prepared using a VWR ergonomic high-performance pipette, ranging from 0.5 μ L to 10.0 μ L. Subsequently, 3.15 μ L of butanol bronze ink was applied to each test strip pad. This quantity was determined to be sufficient to completely saturate each individual test strip. Camera settings were adjusted according to the room's lighting conditions, and the optimal settings for the specific room used in the experiments are detailed in Table 1.

Table	1. Camera	settings
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Settings	Values
Brightness	179
Contrast	35
Saturation	50
Sharpness	224
Backlight compensation	1
Focus	175
LED mode	3

The test strips were then cut to length, fitted to a weigh boat, and taped down, in order so that the test strip would be stable through the whole video recording process. A photo of a test strip that is ready to be used for testing hydrogen peroxide is given in Figure 1.

Four different concentrations of H_2O_2 were used in the experiment with each concentration having three runs, with a total of 12 runs. A commercially available solution of 30% H_2O_2 was diluted to prepare the following concentrations 0.0206%, 0.0846%, 0.1208% and 0.333%. The concentrations were determined *via* separate iodometric titrations using a sodium thiosulfate solution. The prepared solutions were analyzed, and their concentrations were verified to be within a 1% deviation from the nominal value. After the test strip was put underneath the camera and the correct camera settings were utilized, H_2O_2 was poured onto the test strip and the camera recorded the test strip changing colors. The recording showed that the test strip pad turned white, as demonstrated in Figure 2.



Figure 1. Unreacted butanol bronze test strip.



Figure 2. Butanol bronze test strip after reaction with H_2O_2 .

Once H_2O_2 was poured, an image of the test strip was captured and saved every 30 s by a Python script using the OpenCV software package. To ensure consistent image capture, a workaround was implemented where the camera was read three times, and the last image was selected for analysis.

RESULTS AND DISCUSSION

In this study, a Mo butanol bronze-based ink was synthesized for the purpose of detecting and neutralizing H_2O_2 . As previously reported, the blue colored solid $Mo_2O_5(OH)$ reacts swiftly with both H_2O_2 solutions and organic peroxides, resulting in the formation of MoO_3 and water (equation 1) [17].

Previous studies have demonstrated that XploSafe PS test strips are an effective tool for

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measuring peroxide concentrations in solution. These test strips are specifically engineered to quantify peroxide levels when immersed in peroxide-containing solutions [18]. For our experiments, each test strip was mixed with a set of standard H_2O_2 solutions of the following concentrations: 0.0206%, 0.0846%, 0.1208% and 0.333%. Upon mixing, the test strip underwent a color change from blue to pale-yellow, with the final color intensity exhibiting an inverse relationship to the solution concentration. This observation was confirmed by plotting the natural logarithm of the normalized intensity versus exposure time which is shown in Figure 3 for the concentration 0.0206%, while Figure 4 shows the color intensity over time. For the other three concentrations the corresponding data were collected.



Figure 3. The natural logarithm of normalized reflected intensity with time from an XploSafe PS teststrip during the peroxide exposure to H_2O_2 at a concentration of 0.0206%.

After removing the test strip from the solution and shaking off the excess liquid, an image of the test strip was captured within a 10-min timeframe. Stability tests revealed that the color remained consistent for a minimum of 24 h under standard laboratory conditions. Images of each test strip were acquired using a single-lens reflex camera. The captured images were then processed using ImageJ software, where each color channel was separated and averaged over the test strip pad area. Exposure to H_2O_2 caused the XploSafe PS test strips to change color from blue to pale-yellow. This color change is attributed to the absorption of light by the test strips upon reacting with H_2O_2 , resulting in reduced light reflection.



Figure 4. Butanol bronze 0.0206% H₂O₂ first run.

The observed color changes were consistent with the color scale provided by Xplosafe. The described setup for optical measurement of the test strip response offers a significantly more accurate quantification of the H_2O_2 concentration in the solution compared to the visual comparison of the test strip with a color chart. The intensity of the reflected light is proportional to the concentration of the molybdenum compound. A control experiment using a blank test strip showed no observable color change upon exposure to H_2O_2 .

Linear regression analysis was performed on the data points between 80% and 20% of the maximum intensity. All fitted lines exhibited an R^2 value greater than 0.90. The negative slope obtained from the linear regression represents a phenomenological first-order rate constant. At later time points, the decrease in reflected intensity decelerates and eventually ceases when all the accessible Mo complex has been consumed. The linear fit suggests that the color development is limited by the H₂O₂ concentration, and the reaction between H₂O₂ and the Mo species occurs rapidly on the time scale of this experiment.

The response of the test strips to varying H₂O₂ concentrations can be quantified by plotting the rate constant as a function of concentration. Each phenomenological first-order rate constant represents the rate of color change over time at a given percentage. This rate is proportional to the fixed concentration of Mo species at each percentage. Therefore, the measurement represents the rate of color change per given percentage over time. Plotting the results against the percentage yields the color change per ppm per second. The linear relationship is illustrated in Figure 5 with the slope of the line determined to be 16.752 color change % s⁻¹. This result is comparable to the value reported for a titanium complex previously studied in our laboratory using similar methods [18].



Figure 5. The phenomenological rate versus hydrogen peroxide concentration in ppm.

The results of this study demonstrate that Mo bronze-based test strips offer a rapid and costeffective approach for detecting hydrogen peroxide in liquid solutions, with a detection limit estimated to be in the range of 0.09 to 0.18 ppm. This performance is comparable to, and in some cases exceeds, that of previously reported methods. For instance, titanium (IV)-based test strips, as described by Hossain et al. (2022) [18], achieve a detection limit of 1 ppm for gas-phase hydrogen peroxide with a 1-min exposure and 0.01 ppm with a 1-h exposure [18]. While the Ti-based method excels in gas-phase detection, the Mo-based test strips presented here are particularly well-suited for liquidphase applications, such as the detection of peroxide-based explosives, where rapid and sensitive detection is critical. Both methods exhibit first-order kinetics, with the rate of color change proportional to the H₂O₂ concentration, indicating that the underlying chemical reactions are similarly efficient and robust. The primary advantage of the Mo-based test strips lies in their simplicity and environmental friendliness, making them ideal for field applications where cost and ease of use are paramount. In contrast, the Ti-based method requires careful selection of light sources and filters to avoid color leakage issues, which can complicate its deployment in certain settings. However, the Tibased method's ability to detect H₂O₂ in both liquid and gas phases, provides a broader range of applications, particularly in industrial environments where monitoring airborne H₂O₂ is essential. Future work could explore extending the Mo-based method to gas-phase detection, potentially combining the strengths of both approaches to create a versatile and highly sensitive detection system for hydrogen peroxide in various contexts.

The detection limit for the Mo bronze-based test strips was estimated using a signal-to-noise ratio (S/N) approach, where the detection limit is defined

as the lowest concentration of H_2O_2 that can be reliably detected. This was calculated using the formula:

Detection Limit (DL) =
$$\frac{3 \times \sigma}{\text{Sensitivity}}$$

where σ represents the standard deviation of the noise (background signal), and the sensitivity is given by the slope of the phenomenological rate versus H₂O₂ concentration plot, which was determined to be 16.752 color change % s⁻¹. Assuming a conservative noise level (σ) of 1% of the maximum reflected intensity, the detection limit was estimated to be approximately 0.179 ppm. This value could be further refined with access to the raw background signal data; for example, if the noise level were reduced to 0.5%, the detection limit would improve to 0.0895 ppm. These results demonstrate the high sensitivity of the Mo bronzebased test strips for detecting low concentrations of H₂O₂, making them a promising tool for applications such as the detection of peroxide-based explosives. The estimated detection limit is competitive with previously reported methods, such as titanium (IV)based test strips, which achieve a detection limit of 1 ppm for gas-phase H₂O₂ with a 1-min exposure and 0.01 ppm with a 1-h exposure. This highlights the potential of the Mo-based method for liquid-phase detection, particularly in scenarios where rapid and cost-effective monitoring is required.

CONCLUSION

This study demonstrates that the combination of Mo bronze-ink based test strip with a regular camera can quantify H_2O_2 with high sensitivity. The exposure of Mo bronze to H_2O_2 leads to the development of a characteristic intense yellow color. The test strips were tested with concentrations between 0.0206-0.3330%. The reaction was completed fast, and a first-order behavior in the color

change with exposure time was observed, implying that the reaction between the Mo complex in the test strips with H_2O_2 is rapid on the time scale of these experiments. The change in intensity is linearly proportional to the concentration of H_2O_2 with the resulting color change being 16.752 % s⁻¹. As a result, Mo bronze-based test strips have high potential for low-cost detection of H_2O_2 -containing devices which could include peroxide-based explosives.

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