Smart Standards: Demonstration of Thermochromic Inks in Trace Explosive Metrology

NIST scientists have demonstrated the use of thermochromic inks as interactive metrological tools, which can provide "smart" functionality to standard materials now being developed to test the reliability of thousands of trace explosive detectors deployed at airports by the Transportation Security Administration.

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A "smart" standard will respond interactively with changes in its environment in a functional and predictable manner. These changes may include (but are not limited to) temperature, strain, light, and atmospheric pressure. Smart standards can offer levels of performance beyond those of ordinary standards, in that they offer important operational feedback to a user or instrument that can validate and/or adjust reference values of the process.

Thermochromic inks, which respond either reversibly or non-reversibly to temperature changes, have many practical applications. Reversible thermochromics are widely used as safety devices. They are used on engine parts, fire-resistant doors, and saucepan handles to prevent burns by warning of dangerously high temperatures. Non-reversible thermochromic inks have been used to indicate the maximum temperature which has been experienced by (for example) aluminum gas cylinders or in food packaging. The objective is to produce an historical marking system which will change color irreversibly if the object is at any time stored at too high a temperature. A wide range of thermochromic inks with different temperature transitions has been developed, many in the form of polymers whose response can be adjusted by chemical modification.

This year we have demonstrated the use of thermochromic inks as interactive metrological tools, which can provide "smart" functionality to standard materials now being developed to test the reliability of thousands of trace explosive detectors deployed at airports. These detectors utilize thermal desorbers to volatilize residues sampled on a swipe, and the temperature experienced by the residue during desorption is critical to the sensitivity of the trace detection process. Lower temperatures may fail to vaporize the explosive, whereas higher temperatures may cause decomposition. Either result may lead to negative detection of the targeted explosive.

The challenge was to spatially distribute a thermochromic ink across a swipe in a precisely positioned array of visible lines or dots, and yet in minute quantities that would not interfere with the normal operation of a trace explosive detector. Several irreversible inks with color transitions (black-to-red and green-to-red) temperatures between 160 ºC and 200 ºC were procured from Chemsong, Inc. (Chicago, IL). We initially worked with researchers at the University of San Diego (La Jolla) and Großerkmannsdorf, Germany, who have experience in producing intricate arrays on piezoelectric nanoplotters. We were successful in producing arrays of thermochromic inks on several types of swipe media used by manufacturers of trace explosive detectors. Optical microscopy was performed to visualize these thermochromic ink applications, and an example is illustrated in the figure.

Figure One:

Thermochromic ink plotted as lines (ca. 0.3 mm width) on woven PTFE media used by GE Security.

At NIST, we have compared the use of calligraphy pens, rubber stamps, and inkjet printers to produce test swipes that have thermochromic functionality.

These ink types were tested on several IMS-based explosive analyzers to establish ink quantities that would not interfere with explosive detection. This quantity corresponded to about 1.0 µL of undiluted ink, applied across the pattern and well dried. For an array of 100 spots, this is 10 nL per spot. We found that only inkjet printers could reliably deposit these small quantities, which amount to a limit of 200 droplets of diluted (1:1) ink per spot using 58 µm diameter droplets.

While manufacturers of detectors indicate the general location of the optimal area (the "sweet spot") on supplied swipes, the actual location, area, and shape of the true "sweet spot" in a particular detector may be somewhat variable. We designed a pentagonal star-shaped pattern (Fig. 2) that has an inner perimeter surrounding the deposit of trace standard material (not visible). Dotted lines radiate to an outer perimeter, which is about 2.5 cm in diameter and outside the heated area. Upon inspection, the user can verify that the inner perimeter (and sample) was heated to the proper temperature, and trace around the color change limit on each radial line to determine the symmetry of the isotherm.

Future Plans: We anticipate that thermochromic inks will be useful in "smart standard" designs, and add value to many testing & evaluation materials. These inks may be printed on media surrounding deposits of standard materials, in order to verify that the target area achieves a specified temperature during thermal desorption. This will also provide a visible indicator for one-use-only media, and indicate whether the media had been improperly stored in a hot environment prior to use. We will investigate formulating thermochromic inks with non-toxic and biodegradable solvents such as ethyl lactate to provide an environmentally benign inkjet fluid.

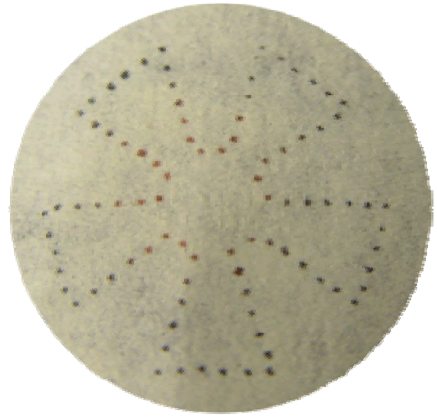

Figure 2: ***On a swipe, a pentagonal star-shaped pattern of thermochromic microdots is used to test the thermal desorption performance of a trace explosive detector. Here, microdots that reached 200 °C during desorption changed color from black to red, confirming adequate performance.***

Report: ***Demonstration of Irreversible Thermochromic Inks in Trace Explosive Metrology***, 837-57-06 to the Transportation Security Administration, NIST Office of Law Enforcement Standards, and the Department of Homeland Security.