SAW Chemical Microsensor Arrays

For weapons proliferation detection

Overview

Sandia National Laboratories' Microsensors S&T Dept. is developing a chemical microsensor-based system to detect the chemical signatures of the production of the weapons of mass destruction (WMD). This program encompasses two key areas of new technology R&D: (1) development of new chemically selective thin-film materials to detect WMD proliferation signatures, with present emphasis on self-assembled monolayers (SAMs), plasma-processed films (PGFs), dendrimeric polymers, and high-area metals and oxides; (2) development of a surface-acoustic wave (SAW)-based microsensor array and associated pattern recognition (PR) algorithms, based on multidimensional cluster analysis, having the capacity to identify and quantify the chemical signatures of production. Using our six-SAW arrays, our PR algorithms have demonstrated identification of 14 different organic compounds and 21 chemical mixtures over a wide concentration range with > 95% accuracy. In addition to immediate needs in WMD proliferation detection, much of this technology will be applicable to chemical microsensors in general, with the ultimate goal of transfer to the private sector to address dual-use applications such as environmental monitoring/remediation, industrial process control, personal health and safety, and vehicle pollution monitoring and control systems. Much of this program is funded through DOE's Office of National Security and Nonproliferation, Office of R&D (NN-20).

Operational Concept

SAW devices are extremely sensitive to tiny mass changes, detecting 100 pg/cm2 – less than 1% of a monolayer of carbon atoms. Our SAW devices use piezoelectric quartz as a substrate; they operate in the 100-MHz regime, relying on two interdigital transducers to launch and detect a wave that travels from one end of the device to the other (Figure 1).

Each transducer is comprised of many pairs of photolithographically defined fingers, each finger only a few micrometers wide.

When coated with a chemically selective thin film, the SAW device is rendered sensitive to chemicals that interact with the film. Figure 2 shows schematically the interaction between a promising new thin-film material, the self-assembled monolayer, and diisopropylmethylphosphonate (DIMP), a simulant for some of the most common CW agents.

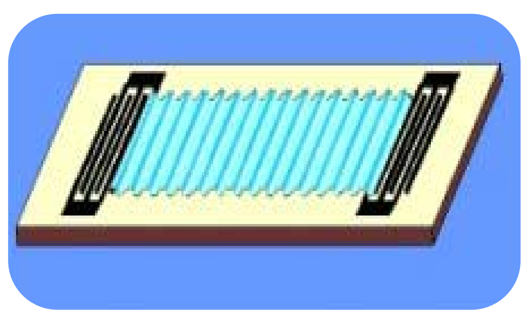

Figure 1. SAW device showing propagating acoustic wave; chemically sensitive coating occupies the region between transducers.

In general, the synthesis or selection of a perfectly selective coating for each analyte of interest is impractical, particularly if large numbers of chemicals are involved. We have demonstrated the use of SAW-device arrays, each bearing a different sensitive film, in combination with cluster analysis-based pattern recognition of the responses. This approach allows several partially selective films to provide a unique signature for each of many compounds or mixtures.

Results

- Combination of the appropriate self-assembled monolayer film (Figure 2) with a SAW device results in a chemical microsensor that distinguishes between chemical weapons stimulants such as DIMP and common interferants such as organic solvents and water.

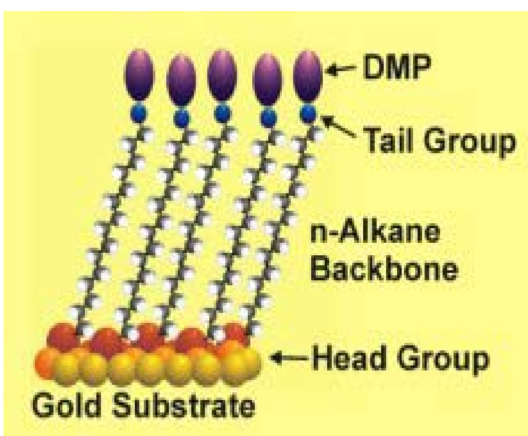

Figure 2. Reversible interaction between se assembled monolayer and CW simulant DIMP.

- A six-SAW-device array was designed and fabricated at SNL, along with the flow control and data acquisition hardware and software required for its operation. In addition to providing six-sensor array data, this system speeds the screening of new coating materials significantly.
- Multidimensional cluster analysis software has been adapted by SNL's Vision Science Dept. for chemical sensor array data analysis with impressive results: using the six-SAW array in combination with both self-assembled monolayers and plasma-grafted polymer films, we have identified each of 14 different organic compounds (listed below) over a wide concentration range with 98% accuracy, and 21 binary mixtures of 7 of these compounds are recognized with 96% accuracy.
- We have also demonstrated reliability of the cluster analysis algorithms in the presence of substantial errors in sensor array calibration, such as could occur with aging of chemically sensitive thin films: individual compounds are still identified with 92% accuracy in the presence of random calibration errors of as much as 25%.
- Species that have been distinguished fall into the general categories of organophosphonate (DIMP, DMMP); chlorinated hydrocarbon (CCl_4, TCE); ketone (acetone, MEK); alcohol (methanol, n-propanol, pinacolyl alcohol); aromatic hydrocarbon (benzene, toluene), saturated hydrocarbon (n-hexane, cyclohexane, i-octane); and water.

For additional information or questions, please email us at MGA@sandia.gov.