Coding and computers help spot methane, explosives

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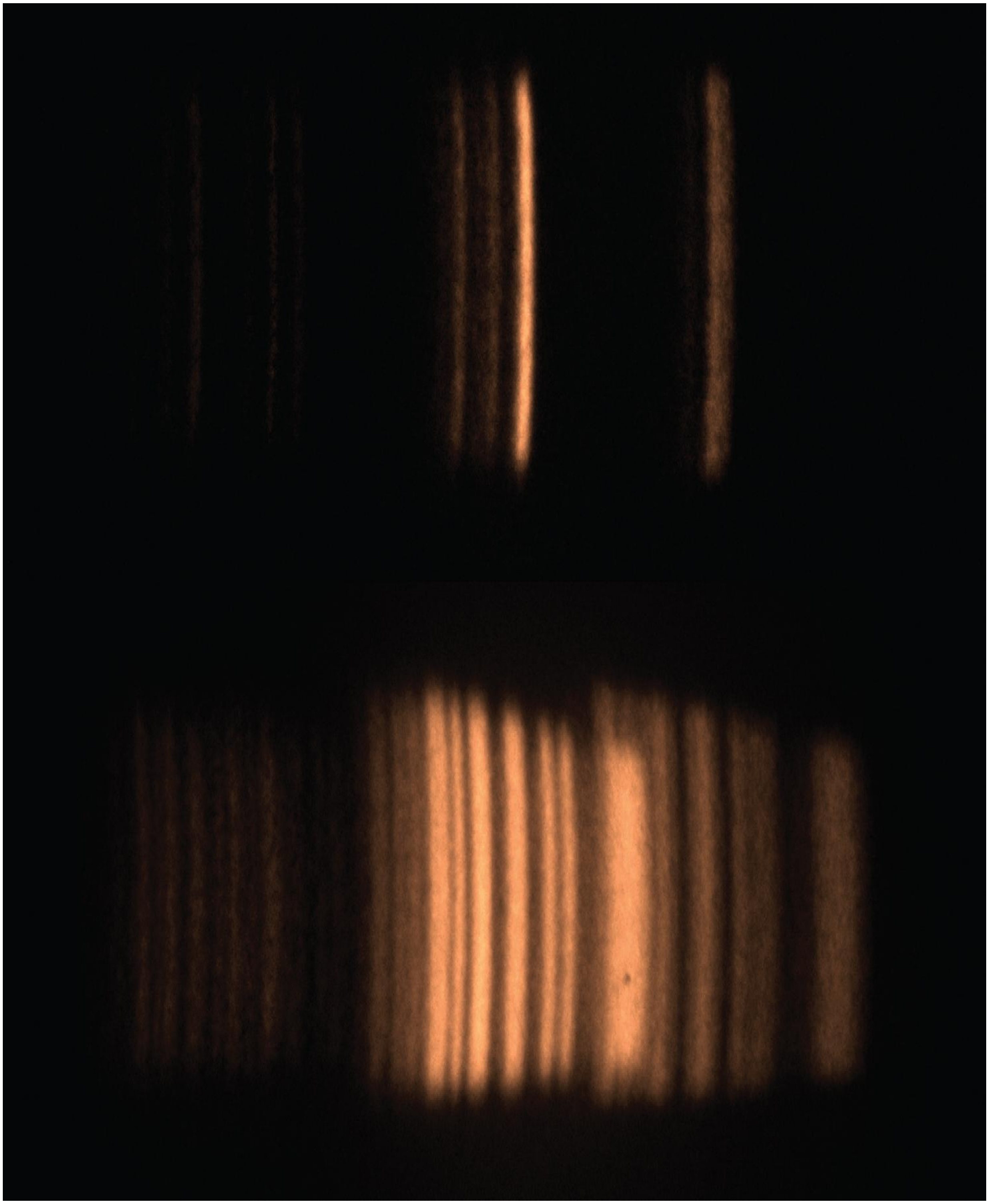

The top image shows a typical reading from a mass spectrometer, where each line indicates the presence of a certain substance. The bottom image shows a reading from the new coded aperture, where researchers rely on computers to collapse the numerous lines into a brighter version of the image above. Credit: Jeff Glass, Duke University

A modern twist on an old technology could soon help detect rogue methane leaks, hidden explosives and much more. A Duke University team is using software to dramatically improve the performance of chemical-sniffing mass spectrometers.

Conventional mass spectrometers separate compounds by giving them an electric charge and passing them through electric and/or magnetic fields. The lighter the compound, the more it bends in the field. By determining what compounds make up a given sample, these instruments can identify almost any substance.

Mass spectrometers were invented in the 1930s, and they're still typically the size of an oven or refrigerator. Inherent hurdles to miniaturization have made it difficult to use them outside of a laboratory. But with the help of modern data analytics, researchers at Duke have demonstrated a technology using a so-called "coded aperture" that promises to shrink these devices while maintaining their performance. The advance could lead to portable mass spectrometers that could be used to detect environmental or safety hazards in the field.

The innovation is featured on the cover of the April issue of the *Journal of Mass Spectrometry*.

"In a typical mass spectrometer, the charged molecules pass through a thin slit, which defines your resolution," said Jeff Glass, professor of electrical and computer engineering at Duke and principal investigator for the project. "When you try to shrink the instrument, you have to shrink the slit too. That means the number of ions (charged molecules) passing through is going to drop and you're going to lose signal intensity. We got around this issue by using a several slits, which code the ions."

Glass likens the new technology to watching a solar eclipse in grade school. Students often poke a small hole in a piece of cardboard, which acts like a lens to create an image of the eclipse on the ground. And as anyone who has ever done this knows, the smaller the hole, the better the detail of the eclipse.

But a smaller hole also makes it dimmer and harder to see. This is exactly the challenge faced when scaling down a mass spectrometer.

The solution, Glass says, is to make many tiny pinholes to create an array of eclipses, and then to use a computer to reconstruct them into a single image. This way you get the sharpness of the tiny pinhole with the brightness of a large pinhole.

The key is in knowing the pattern—or code—of the array of apertures. Thus the name of the technology, coded aperture.

"This idea was actually mentioned in a short article from 1970," said Jason Amsden, a research scientist and manager of the project. "But nobody since then has had all the parts to put it together."

The team drew on several different kinds of expertise. "Our group could do the fabrication of the microstructures, but we relied on engineering colleagues David Brady and Mike Gehm for the coding and computational aspects, and our colleagues at RTI International (in the nearby Research Triangle Park) for the electronics."

The researchers have demonstrated that their coded aperture works in a newer, more complex type of mass spectrometer created to help make the devices smaller, though not nearly as small or precise as coded apertures could make them. Previous papers by the Duke researchers have also shown that the approach improves the performance of very simple mass spectrometers, like those used in the early days of mass spectrometry.

Their work now is focusing on trying coded apertures in different versions of mass spectrometers to determine which would be best for creating scaled down, mobile devices for field use. They are also working to show these devices can detect trace amounts of methane to spot leaks in infrastructure and various explosives to thwart terror attempts.

But the technology can also have an immediate impact in research laboratories around the world.

"This technique can improve the performance of classic mass spectrometers that already have a higher resolution than other types invented for scaling down," said Amsden. "And there are lots of them. Duke alone probably has at least 50 for medical applications. So we're hoping this can have a wide impact in the near future."

More information: Zachary E. Russell et al. Compatibility of Spatially Coded Apertures with a Miniature Mattauch-Herzog Mass Spectrograph, *Journal of The American Society for Mass Spectrometry* (2016). DOI: 10.1007/s13361-015-1323-7

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