New technique can detect structure of promising semiconductor material MoS2

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(Phys.org) —In 2010, the discoverers of graphene—a revolutionary material made of a carbon "monolayer" just one atom thick—snagged the Nobel Prize in physics. An extremely efficient conductor of heat and electricity, graphene could be manufactured with nothing more extraordinary than scotch tape and a pencil. But because it was such a great conductor of electricity, the one-atom-thick material couldn't be used for semiconductors: It lacked a "band gap" that could be used to control the flow of electrons.

"Immediately people identified that graphene had many great properties, but it had no band gap," said Hui Zhao, associate professor of physics and astronomy at the University of Kansas. "Because it had no band gap, you couldn't use it for logic electronics, like computers. You can't turn it off. So people began to look at other materials with similar structures, but those not made of carbon atoms."

Interest turned toward atomically thin molybdenum disulfide, or MoS_2, a layered, black crystalline material with many similarities to graphene, but also possessing a band gap that qualified it for applications as a semiconductor.

Indeed, MoS_2 is seen as an ideal material for a new generation of flexible electronics, said Zhao, such as clothing with photovoltaic properties.

The KU researcher said MoS_2 could even be made in the same way that the discoverers of graphene produced their material, with everyday supplies.

"You can use Scotch tape from Wal-Mart and buy a $100 crystal," said Zhao. "You stick the Scotch tape on the crystal and peel it off. You'll have many flakes on the tape, and usually these are many atomic layers thick. But if you fold the tape and peel again, and do it 10 times, eventually you'll have some flakes that are a monolayer. You'll have a thousand small flakes, but only a few are monolayer—so the trick is to find them. So you put the tape against a substrate of silicon oxide, and then find the monolayers with a microscope."

A more practical technique for making MoS_2 called "chemical vapor deposition," holds the potential to mass-produce the material on a commercial scale. However, the question of how to verify the integrity of the lattice-like structure of monolayer MoS_2 still has been problematic.

Now, Zhao and colleagues have developed a new technique to noninvasively detect the orientation of MoS_2 crystals, as well as the uniformity of their thickness, how their layers are stacked and their single-crystal domain size. The detection technique is known as "second harmonic microscopy."

"It's a conversion of the color of light," said Zhao. "Light is an electromagnetic wave, and different color of light oscillates at different frequency. Usually, for most materials, if you shine a light on them of a certain color, you'll get the same color of light reflected back. But for other materials, if the light is bright enough, then in certain materials, you'll get a different color of light reflected back. If you send in red light, you can get blue light out."

Such is the case with MoS_2. By analyzing the change in light color, researchers are able to detect the structural nature of the material.

"Compared to currently used nonlinear optical materials, such as gallium arsenide crystals, the new material is about 10,000 times more efficient in generating the second harmonic," said Zhao. "We also found that the effect only exist in films of odd number of atomic layers. When there are two or four atomic layers, the effect disappears. This is due to the different symmetric properties of these films. When the film has an even number of atomic layers, it has inversion symmetry. As the name suggests, the inversion symmetry means that the crystal is unchanged after inversion. To understand this, just imagine that one could merge into a crystal and stand at a certain location. When looking forward, one would see a certain arrangement of atoms forming the crystal. If one sees the same arrangement when looking backwards, the location is called a 'center of inversion' for this crystal, and a crystal containing such locations is called inversion symmetric. In such crystals, the second harmonic generation is forbidden. A sample of MoS_2 with two atomic layers is inversion symmetric. Because of that, the effect generated in one layer is perfectly canceled by the other layer. While in monolayers or trilayers, the inversion symmetry is broken, allowing second harmonic generation."

Zhao developed the second harmonic microscopy technique using optical systems in KU's Ultrafast Laser Lab, where previous achievements include breakthrough research on semiconductor "spintronics" and development of a new method of detecting electric currents.

The optical measurement was carried out by KU graduate students Nardeep Kumar, Qiannan Cui and Frank Ceballos, supervised by Zhao. They collaborated with graduate student Sina Najmaei and professors Pulickel Ajayan and Jun Lou from the Department of Mechanical Engineering and Materials Science at Rice University.

The findings on MoS_2 were published this month in the peer-reviewed journal *Physical Review B*. The National Science Foundation, The Kansas Technology Enterprise Corporation and the Welsh Foundation supported the investigation.

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