Researchers find way to tune thermal conductivity of 2-D materials

October 21 2016

Researchers have found an unexpected way to control the thermal conductivity of two-dimensional (2-D) materials, which will allow electronics designers to dissipate heat in electronic devices that use these materials.

2-D materials have a layered structure, with each layer having strong bonds horizontally, or "in plane," and weak bonds between the layers, or "out of plane." These materials have unique electronic and chemical properties, and hold promise for use in creating flexible, thin, lightweight electronic devices.

For many of these potential applications, it's important to be able to dissipate heat efficiently. And this can be tricky. In 2-D materials, heat is conducted differently in plane than it is out of plane.

For example, in one class of 2-D materials, called TMDs, heat is conducted at 100 watts per meter per Kelvin (W/mK) in plane, but at only 2 W/mK out of plane. That gives it a "thermal anisotropy ratio" of about 50.

To better understand the thermal conduction properties of 2-D materials, a team of researchers from North Carolina State University, the University of Illinois at Urbana-Champaign (UI) and the Toyota Research Institute of North America (TRINA) began experimenting with molybdenum disulfide (MoS2), which is a TMD.

The researchers found that, by introducing disorder to the MoS2, they could significantly alter the thermal anisotropy ratio.

The researchers created this disorder by introducing lithium ions between the layers of MoS2. The presence of the lithium ions does two things simultaneously: it puts the layers of the 2-D material out of alignment with each other, and it forces the MoS2 to rearrange the structure of its component atoms.

When the ratio of lithium ions to MoS2 reached 0.34, the in-plane thermal conductivity was 45 W/mK, and the out-of-plane thermal conductivity dropped to 0.4 W/mK- increasing the material's thermal anisotropy ratio from 50 to more than 100. In other words, heat became more than twice as likely to travel in plane—along the layer, rather than between the layers.

And that was as good as it got. Adding fewer lithium ions made the thermal anisotropy ratio lower. Adding more ions also made it lower. But in both cases, the ratio was affected in a predictable way, meaning that the researchers could tune the material's thermal conductivity and thermal anisotropy ratio.

"This finding was very counter-intuitive," says Jun Liu, an assistant professor of mechanical and aerospace engineering at NC State and co-corresponding author of a paper describing the work. "The conventional wisdom has been that introducing disorder to any material would decrease the thermal anisotropy ratio.

"But based on our observations, we feel that this approach to controlling thermal conductivity would apply not only to other TMDs, but to 2-D materials more broadly," Liu says.

"We set out to advance our fundamental understanding of 2-D materials, and we have," Liu adds. "But we also learned something that is likely to be of practical use for the development of technologies that make use of 2-D materials."

More information: Gaohua Zhu et al, Tuning thermal conductivity in molybdenum disulfide by electrochemical intercalation, *Nature Communications* (2016). DOI: 10.1038/NCOMMS13211

Provided by North Carolina State University