Researchers develop novel atom-thin material heat test

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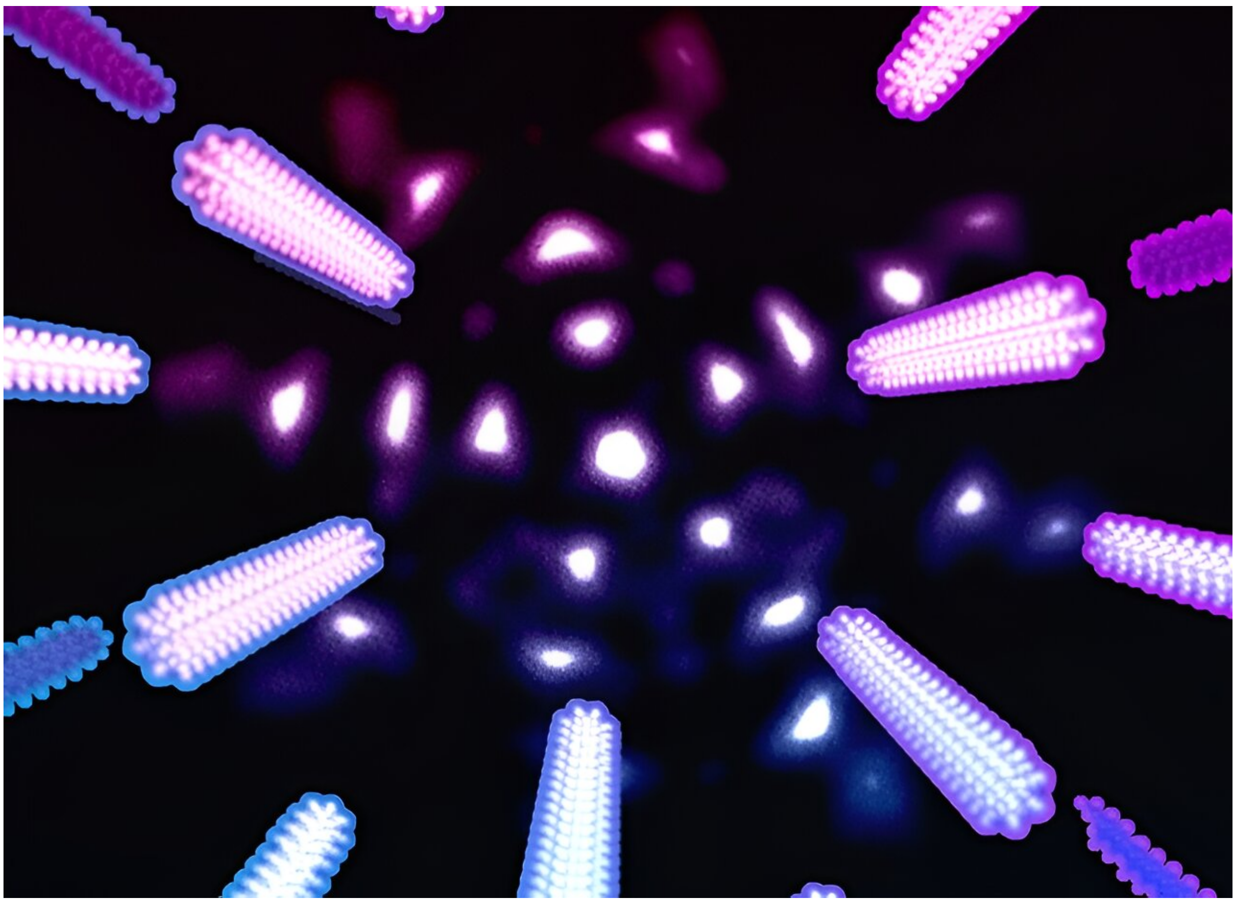

Patterned electron probes yield an extra level of precision in measuring tungsten diselenide lattice parameters. The complex-shaped electron probe is depicted in the background, and exaggerated changes in experimentally observed diffraction peaks due to temperature-induced lattice expansion are depicted in the foreground. Credit: Los Alamos National Laboratory

Advanced materials, including two-dimensional or "atomically thin" materials just a few atoms thick, are essential for the future of microelectronics technology. Now a team at Los Alamos National Laboratory has developed a way to directly measure such materials' thermal expansion coefficient, the rate at which the material expands as it heats.

That insight can help address heat-related performance issues of materials incorporated into microelectronics, such as computer chips. The study is published in *ACS Nano*.

"It's well understood that heating a material usually results in expansion of the atoms arranged in the material's structure," said Theresa Kucinski, scientist with the Nuclear Materials Science Group at Los Alamos. "But things get weird when the material is only one to a few atoms thick."

Due to the thinness of two-dimensional materials, until now, measuring their thermal expansion could only be accomplished indirectly or with the use of a support structure called a substrate. Those limitations have resulted in large discrepancies in the measurements of the thermal expansion.

By using four-dimensional scanning transmission electron microscopy in their experimental setup, paired with a non-circular electron beam and complex computational analysis, the team accurately determined thermal expansion in the material.

Understanding heat in microelectronics materials

Microelectronics, including computer chips, are tiny-scale electronics that rely on semiconducting material, such as the tungsten diselenide on which the team experimented.

Given the advances in materials and architectures required by emerging microelectronic devices, and the production of heat that occurs in any such device, key properties such as thermal expansion of the constituent two-dimensional materials need to be finely understood.

The team grew the tungsten diselenide using a metal-organic chemical vapor deposition, a technique that uses heat to combine gases and leave a deposit of materials only three atoms thick across a 2-inch-diameter glass surface.

The thin film sample was heated to more than 1,000 degrees Fahrenheit while undergoing the 4D electron microscopy experiment—whose tens of thousands of diffraction patterns produced a data set that, when run through a computational analysis, statistically reveal the nature and extent of the changes to the material's structure.

Synthesis methods such as metal organic chemical vapor deposition have a great degree of applicability for fabrication of microelectronics at large scales. Because devices produce heat that can lead to degradation, understanding the thermal behavior of two-dimensional materials fabricated by such techniques—and how it compares to the properties of similar materials in bulk form—helps predict how the material will behave in real application settings under thermal loads.

"Our discovery establishes that the thermal expansion of two-dimensional tungsten diselenide is indeed more in line with the thermal expansion we see in bulk materials," said Michael Pettes, Center for Integrated Nanotechnologies scientist and paper corresponding author.

"This is promising as the value is similar to that of conventional materials used in the existing semiconductors integral to microelectronics."

More information: Theresa M. Kucinski et al, Direct Measurement of the Thermal Expansion Coefficient of Epitaxial WSe2 by Four-Dimensional Scanning Transmission Electron Microscopy, *ACS Nano* (2024). DOI: 10.1021/acsnano.4c02996

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