Boron Nitride and the Nanoribbons of Tomorrow

Materials modeling on ORNL’s ‘Jaguar’ shows big future for boron nitride

Graphene is the current darling of the nanoelectric world. Electrons flow through the material at an astonishing 1 million meters per second, making it a natural for next-generation computer chips, communications equipment and solar energy devices.

But in order to live up to its potential, graphene needs support. On its own, graphene’s edges wrinkle, tear, or roll up—and the silicon dioxide substrate used for today’s microchips is not a good match; its surface is too bumpy and it creates electron-slowing vibrations.

An ideal substrate for graphene would have low electrical resistance and would not physically interfere with the material. “The substrate has to be a dielectric material, a material which is insulating and that can be polarized [positive and negative charges grouped in two distinct regions] by an applied electrical field,” says Alejandro Lopez-Bezanilla, a research associate in ORNL’s Computing and Computational Sciences Directorate.

Lopez-Bezanilla is deep into a computational study of what could be the ideal substrate for graphene—the compound boron nitride.

Boron nitride, like graphene, can be formed as one-atom thick sheets or as nanotubes, then cut into nanoribbons with their atoms arranged in a hexagonal lattice (imagine chicken wire).

After a boron nitride nanotube is cut, the resulting edge shape will affect the behavior of the nanoribbon. A slice straight through the lattice halves every other hexagon, making armchair-shaped edges (aBNNR); zigzagged (zBNNR) edges are made by cuts along the hexagonal borders. The zigzag-cut ribbon has one edge lined with nitrogen atoms and the other with boron atoms. A boron nitride nanoribbon (BNNR) is a quasi-one-dimensional structure, one atom thick, with a width-to-length ratio of 1 to 1,000-plus.

The size of a nanoribbon can be compared with a strand of spider’s silk, which is one thousand times thicker than one BNNR. If the BNNR were scaled up to the thickness of the spider silk filament, a correspondingly scaled silk strand would be as wide as a coin’s edge.

The judicious application of elements to a material—a process known as functionalization—can change the material properties at the nanoscale.
System Overview

- Peak petaflops: 2.33
- Six-core AMD Opteron™ processors: 37,376
- AMD Opteron cores: 224,256
- Compute nodes: 18,688
- Memory (TB): 300
- Disk bandwidth (GB/s): 240
- Disk space (TB): 10,000
- Floor space (SqFt): 5,000

Lopez-Bezaniila pushed boron nitride’s boundaries by modeling the compound under different conditions to see what new properties it might have at the nanoscale, expanding its usefulness. Working with colleagues at ORNL, he simulated zBNNRs modified by oxygen or sulfur atoms attached to each boron and nitrogen atom along the cut edges. Under these conditions, the insulating boron nitride becomes metallic.

The team used two systems for the simulation. Jaguar ran the Vienna Ab-initio Simulation Package (VASP) and the Oak Ridge National Laboratory Institutional Cluster ran the SIESTA code. Both are density functional theory (DFT)-based codes.

“VASP needs the outstanding computational capabilities of Jaguar,” said Lopez-Bezaniila. “To verify the metallic features of the oxygenated zBNNRs with a higher degree of accuracy, we performed spin-polarized calculations with the help of VASP on large unit cells, which needed thousands of processors due to the extensive calculation of large systems at the level of a DFT code based on plane waves.”

Typical job sizes were 2,048 cores. “The project consisted of doing a large number of calculations at different levels of detail,” said team member Bobby G. Sumpter, group leader of Computational Chemical and Materials Science and the Nanomaterials Theory Institute at ORNL. “Jaguar was needed to perform certain calculations that used a different level of detail for the electronic structure—in particular to check system size effects and more rigorous treatment of electron exchange and spin, but also to examine the use of more complete basis sets. Basically Jaguar provides the required computational engine that enables us to do a complete study, without which we would not have been able to fully develop an understanding of the boron nitride nanoribbons within months.”

The computational models showed that the edge shape, the choice of added elements—oxygen, sulfur, or hydrogen—and the location of the elements all play a role in creating different behaviors in the nanoribbons.

The repetitive zigzag edge shape sets the added oxygen atoms at the same position—always parallel to the edge and equidistant from the adjacent oxygen atoms, so that the electron shells overlap, allowing electrons to move between atoms. In other words, it gives the nanoribbon metallic qualities. If BNNRs with armchair edges are modified, the oxygen atoms are arranged differently, preventing the emergence of metallic characteristics.

Both oxygen and sulfur render the zBNNRS metallic, whereas the control group of hydrogen-edged zBNNRs was semiconducting and nonmagnetic.

The placement of the elements also affects the metallic qualities and conductivity. “To show the importance of the edges [in converting] the zBNNRs into a metallic compound, we modeled the doping of the ribbon when the oxygen atoms form an extended wire embedded in the center of the ribbon,” says Lopez-Bezaniila. “The result is that it conserves its insulating features.”

The team outlined its findings in a July 7, 2011, paper in the American Chemical Society journal Nano Letters. The simulation results have not yet been tested in a laboratory.

Simulating the transformation of a known material into one with novel features opens the door to possible new uses—optical, magnetic, electronic. There is a new world of opportunities for the features in zigzag-edged boron nitride nanoribbons.

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