Argonne NATIONAL LABORATORY

News Release

Media Contact: Steve McGregor
(630) 252-5580
smcgregor@anl.gov
For immediate release

'Hybrid' semiconductors show zero thermal expansion; could lead to hardier electronics and optoelectronics

ARGONNE, Ill. (Dec. 19, 2007) – The fan in your computer is there to keep the microprocessor chip from heating to the point where its component materials start to expand, inducing cracks that interrupt the flow of electricity — and not incidentally, ruin the chip. Thermal expansion can also separate semiconducting materials from the substrate, reduce performance through changes in the electronic structure of the material or warp the delicate structures that emit laser light.

Recently published research by scientists at the U.S. Department of Energy's National Renewable Energy Laboratory (NREL) and Argonne National Laboratory, and academic institutions has shed light on a semiconducting material with zero thermal expansion (ZTE). The research may play a role in the design of future generations of electronics and optoelectronics that can withstand a wide range of temperatures.

Traditional interests in ZTE materials have largely been in areas such as optics, heat-engine components and kitchenware. ZTE materials with applications in non-conventional areas such as electronics and optoelectronics are rare; most are glasses, which do not work well in electronics applications. The hybrid inorganic-organic semiconductor investigated in this work is a multifunctional semiconductor that has previously been shown to possess superior electronic and optical properties. The work also suggests an alternative route to designing materials with any desired positive or negative thermal expansion.

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“It’s a merger of inorganic and organic materials,” said Zahirul Islam, a physicist in Argonne’s X-Ray Science Division, “which form a fully coherent, three-dimensionally ordered crystal. Normally inorganic and organic materials don't work very well together, but here they are working together to display these remarkable properties.”

The materials under study form alternating organic and inorganic layers that work together to produce these effects. One contracts while the other expands, and the net effect is zero.

“This work suggests a novel approach to design the thermal expansion — from positive to negative, including zero — in a nanoscopic scale by assembling nano-scale units in an ordered manner,” said principal investigator Yong Zhang of NREL. “The idea has only been demonstrated for tuning thermal expansion in one dimension and study was limited to one or two materials. Next, we would like to extend the idea to higher dimensions (i.e., ZTE in more than one dimension), and explore more inorganic-organic combinations.”

These hybrid materials hold promise for high-efficiency semiconductor lasers, ultrathin and flexible solar cells and light-emitting and detecting devices. It is possible to “dope” the materials (adding small amounts of other compounds) to form transparent conducting materials, Zhang said.

While chemical and thermal stability are two major problems for most hybrids, the hybrid nanostructures investigated in this work are found to be exceptionally stable in the air, even under the illumination of an ultraviolet laser.

“Not only do the crystal structures remain unchanged,” Zhang said, “but their electronic and optical properties remain after a few years of air exposure or upon heating to more than 200 degrees C, a feature attributed to the strong covalent bonding throughout the structure.”

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This work involved multiple institutes with complementary strengths and capabilities. Scientists at NREL initiated and organized the project. The materials were synthesized by Jing Li’s group at Rutgers University. Critical X-ray diffraction measurements to determine the ZTE effects were carried out at Argonne's Advanced Photon Source. Other key Argonne researchers are Yang Ren and Peter L. Lee. Theoretical modeling on the phonon (vibrational) spectrum, crucial to the understanding of the experimental findings, was performed by scientists at the University of Arkansas. Collaborators at the University of Colorado at Boulder also made important contributions to the work.

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