Recipe for oxide interface perfection opens path to novel materials

Oak Ridge National Laboratory

OAK RIDGE, Tenn., Nov. 16, 2012 — By tweaking the formula for growing oxide thin films, researchers at the Department of Energy's Oak Ridge National Laboratory achieved virtual perfection at the interface of two insulator materials.

This finding, published in the journal Advanced Materials, could have significant ramifications for creation of novel materials with applications in energy and information technologies, leading to more efficient solar cells, batteries, solid oxide fuel cells, faster transistors and more powerful capacitors.

The research team, led by ORNL's Ho Nyung Lee, demonstrated that a single unit cell layer of lanthanum aluminate grown on a strontium titanate substrate is sufficient to stabilize a chemically and atomically sharp interface. A unit cell is the smallest group of atoms that possess the properties of a crystalline material.

"This means that we can now create new properties by precisely conditioning the boundary in the process of stacking different oxides on top of each other," said Lee, a member of the Materials Science and Technology Division.

What's especially noteworthy is that a layer even one unit cell thick could serve as a buffer and dramatically improve the interface quality.

For this research, Lee and colleagues used pulsed laser deposition to deposit lanthanum aluminate thin films on strontium titanate substrates. They were able to demonstrate that a mundane variable such as the oxygen pressure during deposition of lanthanum aluminate is the key factor for achieving atomically sharp interfaces and changing the interface properties on a single unit cell level. Importantly, this finding is not limited to fine-tuning this particular interface, but also applies to a broad range of oxide heterostructures in a class of minerals known as perovskites.

The discovery of electrical properties in oxides - ordinarily insulators - has generated excitement and potentially creates the possibility that oxide electronics could become an alternative to the current semiconductor technology based on silicon.

Making this finding possible was Argonne National Laboratory's Advanced Photon Source and the extreme brightness of synchrotrons that allowed scientists to study the structure and composition at the interface.

"The sophisticated surface X-ray diffraction methods available at the Advanced Photon Source were key to zeroing in on the origin of the interface behavior," said

co-author and colleague Gyula Eres.

While previous research with lanthanum aluminate thin film growth used low oxygen pressures, Lee and colleagues systematically explored the effects of oxygen pressure in a wide range. They determined that a shielding layer of lanthanum aluminate grown at high oxygen pressure followed by continued growth at a lower pressure resulted in a highly ordered atomically and chemically sharp - essentially defect-free -- interface.

Other ORNL authors of the paper, titled "Atomic Layer Engineering of Perovskite Oxides for Chemically Sharp Heterointerfaces," are Woo Seok Choi, the first author, Christopher Rouleau and Sung Seok Seo. Other institutions contributing to the paper are the University of Kentucky, Argonne National Laboratory and the University of Science and Technology of China.

Funding for this research was provided by the DOE Office of Science, which also supports the Advanced Photon Source. The Office of Science is the single largest supporter of basic research in the physical sciences in the United States and is working to address some of the most pressing challenges of our time. For more information, please visit http://science.energy.gov/ [1]. UT-Battelle manages ORNL for DOE's Office of Science.

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