

Researchers image atomic structural changes that control properties of sapphires

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Materials scientists from Case Western Reserve University and the Institute of Solid State Research in Julich, Germany have produced particularly clear changes in the atomic structure of sapphire following deformation at high temperatures.

Peering through an electron microscope down to a level where a human hair would seem as wide as a washer and dryer set, they were able to quantify deviations from the regular columns of aluminum and [oxygen atoms](#) - the stuff of perfect sapphire crystals. The work is published in the journal *Science* Friday, Nov. 26.

These structural changes are called dislocations and include very small rearrangements of some of the aluminum atoms from their normal surroundings of six oxygen atoms to a layout of four surrounding oxygen atoms.

While the changes in structure are minute, they deliver a punch.

In the orderly world of crystals, dislocations can control electrical, chemical and [magnetic properties](#) as well as strength and durability. And, the information and imaging technique used in the study can be applied to all crystalline solids, from microchips to thermal protection systems that shield jet engines from extreme heat.

"We imagined this might have been the possible change in structure a year or so ago and now we're able to see how the atoms are moving with

respect to one another," said Arthur Heuer, Distinguished University Professor and Kyocera Professor of Ceramics in the department of materials science and engineering at the Case School of Engineering. "The important thing is we were able to image it with [atomic resolution](#)."

Peter Lagerlöf, an associate professor of materials science and engineering at Case Western Reserve, noted that "understanding the structure of the dislocations is important because it allows increased understanding of material properties."

Heuer traveled to Julich, Germany, where he worked with Chunlin Jia at the Institute of Solid State Research and Ernst Ruska-Centre for Electron Microscopy. There, using an ultra high magnification transmission [electron microscope](#), the scientists employed negative spherical aberration imaging to a section of synthetic sapphire to see dislocation cores.

This is the first time the technique was applied at subangstrom resolution to structural defects in ceramics.

The scientists were able to distinguish columns of oxygen from columns of aluminum in synthetic sapphire, used to make substrates for specialty advanced computer chips (because of sapphire's good thermal conductivity and electrical resistivity), and grocery store scanners and expensive watch faces (because of sapphire's superior scratch-resistance compared to glass).

Dislocation cores terminate with aluminum atoms and electrical neutrality is maintained as the cores occupy only half of the aluminum sites. A complex mix of six-fold and four-fold coordinated aluminum polyhedra are found in the dislocation cores.

Jacques Castaing, a materials scientist at Laboratoire Physique des

Materiaux, CNRS Bellevue, F 92195 Meudon Cedex, France, was not involved in the experiment but with Heuer and Lagerlöf, last year published a theory that the atomic structure would change this way.

Castaing said that being able to see the dislocations, "for the basic knowledge of materials, is very important. These dislocations are everywhere."

Provided by Case Western Reserve University

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