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Researchers develop method to measure positions of atomic sites with new precision

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(Phys.org) —Using a state-of-the-art microscope and new methods in image processing, a multi-institutional team of researchers has devised an inventive way to measure the positions of single atomic sites in materials more precisely than ever before.

In a paper published June 11, 2014 in the journal *Nature Communications*, the team demonstrated the ability to locate atoms in high-resolution images of materials to better than one picometer, or one-hundredth of a nanometer. That is more than five times better than previous imaging methods.

Andrew Yankovich, a materials science and engineering graduate student at the University of Wisconsin-Madison, is the first author on the paper.

The new technique enables researchers to pinpoint previously undetectable shifts of single atomic sites in a material. Insights into these atomic shifts could help pave the way for innovative new materials.

"Before our work, scientists could use X-ray diffraction techniques to measure millions of atoms at a time, and if a whole bunch of those atoms move a little closer or a little farther apart, that shift is measureable," says co-author Paul Voyles, an associate professor of materials science and engineering at UW-Madison.

Although X-ray diffraction is still a better way to measure shifts involving huge numbers of atoms to much higher precision, it doesn't provide useful measurements for particular structures where researchers are trying to measure shifts in only a few atoms.

"Now, with this new technique, we can say 'this atom moved a little closer to that atom—and we are talking about only these two atoms," says Voyles. "That gives us the ability to answer questions about the atomic origin of the function of entirely new classes of materials, like metal nanoparticle catalysts, that were very hard to measure before."

Although Voyles and his team use a state-of-the-art scanning transmission electron microscope (STEM) at UW-Madison to gather experimental data, measuring atomic structures at the picometer scale is extremely difficult, says Voyles.

"If anything moves—the probe beam of electrons, the sample, the microscope itself, or the electric current flowing in any of the lenses—then it adds instability to the image, meaning that atoms move away from where they ought to be in the image," says Voyles. "The STEM is extremely sensitive to the environment that it sits in."

Voyles started this research project because he was looking for a solution to these instrumental instabilities, which limited the ability to make more precise measurements of atomic sites.

Voyles says interdisciplinary collaboration played a crucial role in solving the problem. He met his collaborators at a workshop organized by co-authors Peter Binev and Wolfgang Dahmen at the Interdisciplinary Mathematics Institute at the University of South Carolina, which invited Voyles and others in the field of electron microscopy to talk about challenges in their field. He teamed up with experts in applied mathematics and image processing to look for solutions.

Voyles says the breakthrough came when the team found new and clever ways to combine data science techniques from applied mathematics to work with STEM materials data. The result was a new combination of mathematics and algorithms, built into a software tool.

The new technique involves using the STEM to take about 500 images of a sample as quickly as possible. The images all ought to be the same—but they aren't, because the instabilities can cause atoms to appear in the wrong positions. To correct this, the researchers use an algorithm to estimate all of the instabilities in every image and undo them, yielding corrected images at a new level of precision.

The next steps would be to improve the usability and efficiency of the software and to make it widely available.

"I think there's a big opportunity for continued interdisciplinary collaboration of a similar type to what we've done, to push forward into new answers to scientific questions," says Voyles.

Provided by University of Wisconsin-Madison