

Atomic-level 3D models show us how gadgets work

October 6 2022, by Steinar Brandslet

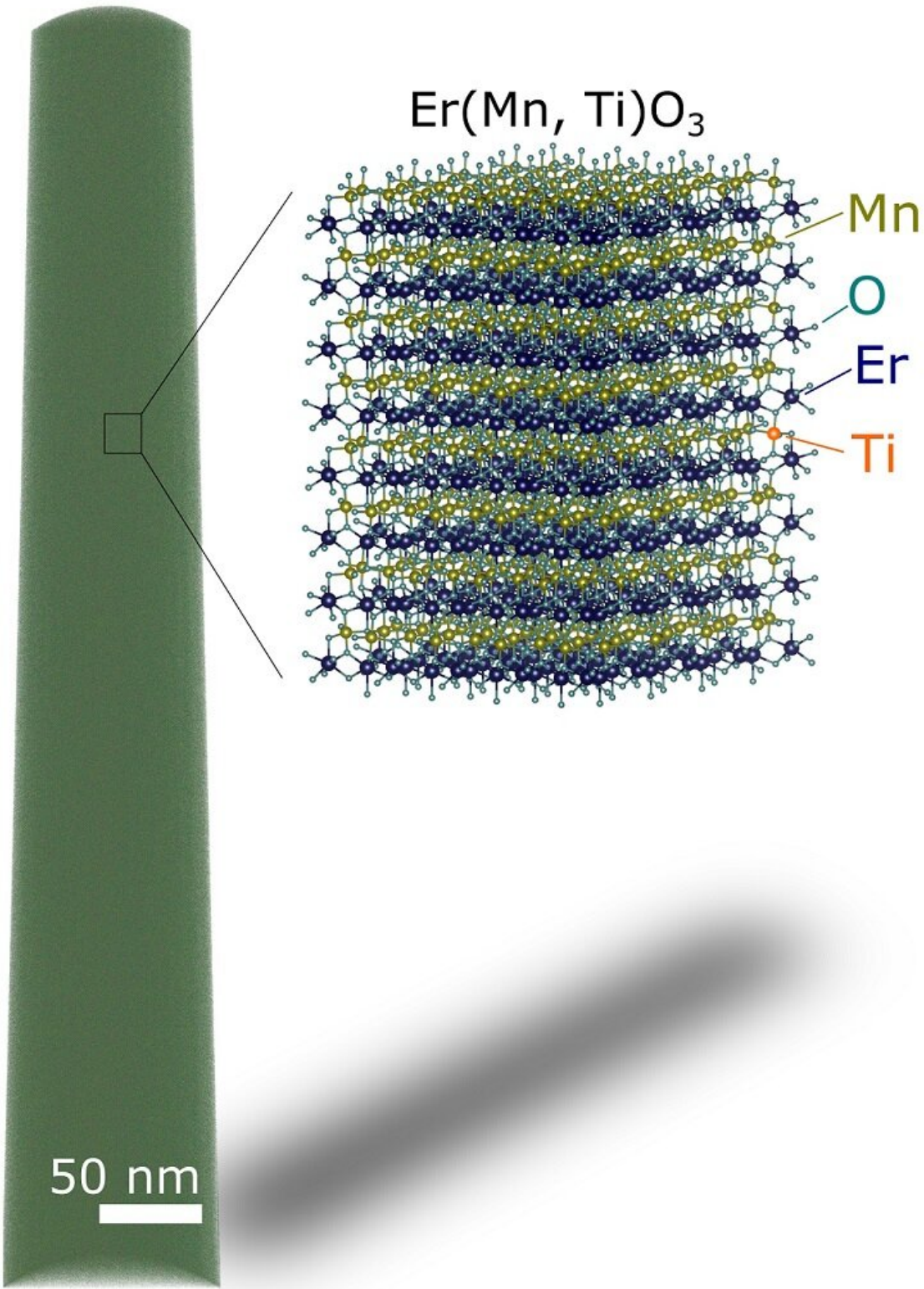


Illustration of atom probe tomography analysis. The 3D map on the left shows the measured distribution of atoms, with each point representing one atom. From the APT data, the researchers can build precise atomic-scale models as shown on the right. They can identify individual atoms, here titanium (Ti), that have been added to the material (ErMnO₃) to tailor its properties. Credit: Kasper Aas Hunnestad, NTNU

Although nanotechnology and materials science are complicated topics for most of us, the research in these fields is of great importance to almost everyone. Your digital gadgets, for example, are completely dependent on it.

Today, all microelectronics depend on semiconductors. These are materials that are not very good at conducting electricity. But you can add tiny amounts of other substances to them, a process known as doping. This improves the semiconductor's performance so they're not so bad after all.

"In the past, we doped semiconductors and saw that this drastically changed the electrical properties of the material," says Ph.D. candidate Kasper Aas Hunnestad at NTNU's Department of Materials Science and Engineering.

This is all well and good. It's nice when something works. But beyond the fact that it works, we haven't always understood very much of why it does. This is especially true at the atomic level.

"Now, we know much better how we can image the individual added atoms, which previously used to be almost impossible to find. This gives us new insight and allows us to understand how they affect that material's properties," says Hunnestad.

Why 'knowing why' is important, too

So what? Why on Earth should we care about single atoms and why something works? Isn't it good enough just to know that it does work? If this was the case, physicists and chemists would certainly have fun doing the research, but the rest of us wouldn't benefit much from it.

"Only when you know more about how something works, can you manipulate the material and optimize it," says Dennis Meier. He is a professor in the Department of Materials Science and Engineering at NTNU, who led the project.

This way, for example, you can make more efficient, environmentally friendly, or cheaper materials for the job to be done. Or you can assign new properties to a material that you already have available with much greater precision. This is also key for developing future materials for sustainable technology.

"Often, we want to introduce new functionality to materials. For that we need to know exactly what role each individual atom plays," says Meier.



The NTNU-SINTEF team. Sverre M. Selbach, Muhammad Zeeshan Khalid, Antonius T. J. van Helvoort, Kasper A. Hunnestad, Constantinos Hatzoglou, Dennis Meier and Per Erik Vullum. Credit: Geir Mogen, NTNU

Advanced imaging techniques make it possible

Hunnestad and colleagues present the results of many, many hours of work using "[atom probe tomography](#)" (APT) in a recent article in *Nature Communications*.

APT is an advanced piece of cutting-edge equipment that NTNU acquired a few years ago. The machine can provide a three-dimensional representation of what a material looks like, right down to the atomic level, explains Constantinos Hatzoglou. He is a senior engineer in the

APT laboratory at the Department of Materials Science and Engineering.

Hunnestad and colleagues utilized this outstanding capability to study a new type of oxide-based semiconductor to which very small amounts of a substance have been added to tailor its properties.

"Conventional microscopy techniques didn't allow us to observe how small amounts of additives positioned themselves in semiconductors," says Hunnestad. The new results show that the investment in the very best technical equipment, such as this APT machine, pays off enormously and makes ground-breaking research possible.

Shows the enormous potential

The research is still not exactly easy using APT either. But by bringing together colleagues with different experimental and theoretical backgrounds—along with hard and inspired work—the NTNU team has found solutions.

"This isn't just a wonderful achievement. It also shows the [enormous potential](#) of the APT technique for research fields where it has not been applied before. It shows the unique opportunities we have thanks to the modern infrastructure available in NTNU's NanoLab and TEM Gemini Center," says Meier.

Hunnestad has worked with APT for about three years. He has carried out extensive correlated microscopy measurements, supported by Antonius van Helvoort and Per Erik Vullum. Van Helvoort is a professor at NTNU's Department of Physics and experts in high-resolution electron microscopy, while Vullum is a professor II at NTNU, Department of Physics and senior researcher at SINTEF Industry.

Hunnestad and Meier are enthusiastic about all the fascinating

possibilities that have already emerged from their APT-based research and the novel perspectives for the characterization of functional materials at the atomic scale.

Imaging of individual titanium atoms mixed into a semiconductor

For their recent article, the research group looked at the oxide-based semiconductor $\text{Er}(\text{Mn},\text{Ti})\text{O}_3$. For this purpose, their collaborators at the Lawrence Berkeley National Laboratory in the U.S. added tiny amounts of the element titanium (Ti) to erbium manganate (ErMnO_3).

"With the atom probe, we can get a three-dimensional representation of how the titanium atoms are positioned in the semiconductor," says Meier. "This allows us to link the new electrical properties of the material all the way down to individual atoms."

Dr. Muhammad Zeeshan Khalid is a member of the team headed by Sverre Selbach, a professor at NTNU's Department of Materials Science and Engineering. He supplemented the experiments with calculations. These calculations provide further insight into the effects that individual atoms can have on the physical properties.

One of the advantages of what the researchers have done is that they can use the method on many other substances as well. It is not just limited to the substances that the research team at NTNU has experimented with.

"The procedures and the results are of broad interest. They can extend our understanding of oxide-based semiconductors and functional materials in general. The research opens completely new doors," Meier says.

Cooperative approach strengthens research

Many people from different departments at NTNU contributed to make this scientific breakthrough possible. SINTEF, the Research Council of Norway, the Norwegian Micro- and Nano-Fabrication Facility (NorFab), the Norwegian Laboratory for Mineral and Materials Characterization (MiMaC), the Norwegian Center for Transmission Electron Microscopy (NORTEM) and NTNU Nano supported the work.

The researchers point out that this collaborative effort nicely showcases the strength of interdisciplinary research. It shows what can be accomplished with a solid start-of-the-art infrastructure.

The details of how Hunnestad achieved such outstanding results are probably not easily digestible for most of us. But the link to the research article below will give you something to chew on if you want to dig in.

More information: K. A. Hunnestad et al, Atomic-scale 3D imaging of individual dopant atoms in an oxide semiconductor, *Nature Communications* (2022). [DOI: 10.1038/s41467-022-32189-0](https://doi.org/10.1038/s41467-022-32189-0)

Provided by Norwegian University of Science and Technology

Citation: Atomic-level 3D models show us how gadgets work (2022, October 6) retrieved 24 July 2024 from <https://phys.org/news/2022-10-atomic-level-3d-gadgets.html>

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