

## A 20-year-old puzzle solved: Researchers reveal the 'three-dimensional vortex' of zerodimensional ferroelectrics

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Three-dimensional polarization distribution of BaTiO<sub>3</sub> nanoparticles revealed by atomic electron tomography. (Left) Schematic of the electron tomography technique, which involves acquiring transmission electron microscope images at multiple tilt angles and reconstructing them into 3D atomic structures.(Center) Experimentally determined three-dimensional polarization distribution inside a BaTiO<sub>3</sub> nanoparticle via atomic electron tomography. A vortex-like structure is clearly visible near the bottom (blue dot).(Right) A two-dimensional crosssection of the polarization distribution, thinly sliced at the center of the vortex, with the color and arrows together indicating the direction of the polarization. A distinct vortex structure can be observed. Credit: Multi-Dimensional Atomic Imaging Laboratory (MDAIL) at KAIST



Materials that can maintain a magnetized state by themselves without an external magnetic field (i.e., permanent magnets) are called ferromagnets. Ferroelectrics can be thought of as the electric counterpart to ferromagnets, as they maintain a polarized state without an external electric field.

It is well-known that ferromagnets lose their magnetic properties when reduced to nano sizes below a certain threshold. What happens when ferroelectrics are similarly made extremely small in all directions (i.e., into a zero-dimensional structure such as nanoparticles) has been a topic of controversy for a long time.

A research team led by Dr. Yongsoo Yang from the Department of Physics at KAIST has, for the first time, experimentally clarified the three-dimensional, vortex-shaped polarization distribution inside ferroelectric nanoparticles through international collaborative research with POSTECH, SNU, KBSI, LBNL and University of Arkansas.

This research was published online in *Nature Communications* in a paper titled, "<u>Revealing the Three-Dimensional Arrangement of Polar</u> <u>Topology in Nanoparticles</u>."

About 20 years ago, Prof. Laurent Bellaiche (currently at University of Arkansas) and his colleagues theoretically predicted that a unique form of polarization distribution, arranged in a toroidal vortex shape, could occur inside ferroelectric nanodots. They also suggested that if this vortex distribution could be properly controlled, it could be applied to ultra-high-density memory devices with capacities over 10,000 times greater than existing ones.

However, experimental clarification wasn't achieved due to the difficulty of measuring the three-dimensional polarization distribution within ferroelectric nanostructures. Now, the research team at KAIST has



successfully solved this 20-year-old challenge by implementing a technique called atomic electron tomography.

This technique works by acquiring atomic-resolution transmission electron microscope images of the nanomaterials from multiple tilt angles, and then reconstructing them back into three-dimensional structures using advanced reconstruction algorithms.

Electron tomography can be understood as essentially the same method used with the CT scans in hospitals to view <u>internal organs</u> in three dimensions; the KAIST team adapted it uniquely for nanomaterials, utilizing an <u>electron microscope</u> at the single-atom level.

Using atomic electron tomography, the team completely measured the positions of cation atoms inside <u>barium titanate</u> (BaTiO<sub>3</sub>) nanoparticles, a well-known ferroelectric material, in three dimensions. From the precisely determined 3D atomic arrangements, they were able to further calculate the internal three-dimensional polarization distribution at the single-atom level.

The analysis of the polarization distribution revealed, for the first time experimentally, that topological polarization orderings including vortices, anti-vortices, skyrmions, and a Bloch point occur inside the zero-dimensional ferroelectrics, as theoretically predicted 20 years ago. Furthermore, it was also found that the number of internal vortices can be controlled depending on their sizes.

Prof. Sergey Prosandeev and Prof. Bellaiche (who proposed with other co-workers the polar vortex ordering theoretically 20 years ago), joined this collaboration and further proved that the vortex distribution results obtained from experiments are consistent with theoretical calculations.

By controlling the number and orientation of these polarization



distributions, it is expected that this can be utilized in a next-generation high-density memory device that can store more than 10,000 times the amount of information in the same-sized device compared to existing ones.

Dr. Yang, who led the research, explained the significance of the results, "This result suggests that controlling the size and shape of ferroelectrics alone, without needing to tune the substrate or surrounding environmental effects such as epitaxial strain, can manipulate ferroelectric vortices or other topological orderings at the nano-scale. Further research could then be applied to the development of nextgeneration ultra-high-density memory."

**More information:** Chaehwa Jeong et al, Revealing the threedimensional arrangement of polar topology in nanoparticles, *Nature Communications* (2024). DOI: 10.1038/s41467-024-48082-x

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