

atmosphere, it will probably be necessary to get a close-up view once again.

Happily for seventh-planet aficionados, a Uranus orbiter and probe was deemed the top-priority flagship mission by the latest planetary science decadal survey, released in April 2022 by the National Academies of Sciences, Engineering, and Medicine. The recommendation alone is no guarantee that

the project will come to fruition, but it bodes well. The top two priorities of the previous survey—a Mars sample-return mission and the *Europa Clipper*—were both funded, with launches planned in the next few years.

For Uranian science, time is of the essence. If launched in 2031 or 2032, a Uranus-bound spacecraft could capitalize on a gravity assist from Jupiter and

reach its destination in a mere 13 years. If launched later, its journey will take much longer.

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References

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Understanding how metal-nitride ferroelectrics switch their polarization

Transmission electron microscopy images and first-principles calculations suggest that the atoms adopt a disordered but low-energy configuration that facilitates the switching.

Studied for more than a century, ferroelectric materials exhibit a spontaneous polarization in one or more directions along a crystal axis. Thermodynamically stable, the polarized states can be switched from one to the other by applying an electric field that exceeds what's known as the coercive field E_c . That switchability provides the basis for the nonvolatile RAMs in computing. (See the article by Orlando Auciello, James F. Scott, and Ramamoorthy Ramesh, *PHYSICS TODAY*, July 1998, page 22.)

Since the 1960s, electrical engineers have been designing memory elements based on conventional ferroelectrics such as the perovskite barium titanate. But manufacture is complicated by the challenge of integrating those materials with silicon-based semiconductors. What's more, the memory elements are difficult to scale down to atomic dimensions for energy efficiency. Between 2019 and 2021, researchers discovered that crystalline films of alloyed aluminum nitride are ferroelectrics that could solve

both problems. Boron-doped AlN, in particular, is easy to integrate, as it consists exclusively of elements common in silicon electronics.

The discovery was a surprise to most scientists. The films were well-known pyroelectric and piezoelectric crystals, but few believed they could be ferroelectric, because their coercive fields are just too perilously close to the field at which the materials experience dielectric breakdown. Apply a high enough electric field to switch the polarization and you risk destroying the material.

Pennsylvania State University materials scientists Jon-Paul Maria, Susan Trolier-McKinstry, and Ismaila Dabo, who had demonstrated ferroelectricity in B-doped AlN two years ago,¹ have now teamed up with Carnegie Mellon University materials scientists Sebastian Calderon and Elizabeth Dickey to address the dielectric-breakdown problem.² The collaborators realized that if they understood the mechanism by which the polarization switches at the

atomic scale, they could manipulate it—for example, by straining the film, growing it thinner, or altering its dopant concentration.

Such tricks may dramatically lower the coercive field from roughly 4–6 MV/cm in metal nitrides down to levels approaching 1 MV/cm. That transformation would render the new ferroelectrics more practical for applications in memory, energy-harvesting, and high-speed and high-power circuits.

Double duty

Fortunately, there are a few ways to ensure that the coercive field is lower than the dielectric breakdown field. At elevated temperatures, the margin separating E_c and the breakdown field increases, for instance.

As deposited on a tungsten electrode, $\text{Al}_{15/16}\text{B}_{1/16}\text{N}$ films grow with a polarization that points downward (into the substrate)—a configuration shown in figure 1a and referred to as N-polar growth. The image depicts the thickness of a film, grown upward from the bottom of the frame. The tetrahedron diagrams show the positions of the metal atoms Al or B (gray) relative to the N atoms (blue). The metal atom in each tetrahedron is bonded to four N atoms.

To experimentally study the films' local structure and polarization, the researchers used scanning transmission electron microscopy (STEM). And in a standard imaging mode known as differ-

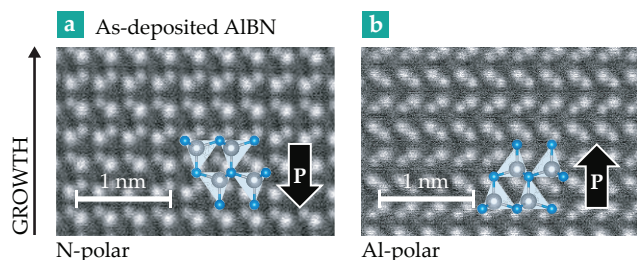


FIGURE 1. BEFORE AND AFTER polarization reversal. These transmission electron microscopy images are on-edge views of a boron-doped aluminum nitride film—a mere 6 nm thick—that show the projections of N, Al, and B atoms through the lattice. **(a)** In AlBN as it's deposited on tungsten, the polarization orientation $\mathbf{P}$ is down, or N-polar. **(b)** After the surface expels enough charge to exceed the coercive field, the polarization flips upward (Al-polar) and the angles between the N atoms and the Al or B atoms change their relative orientation. (Adapted from ref. 2.)

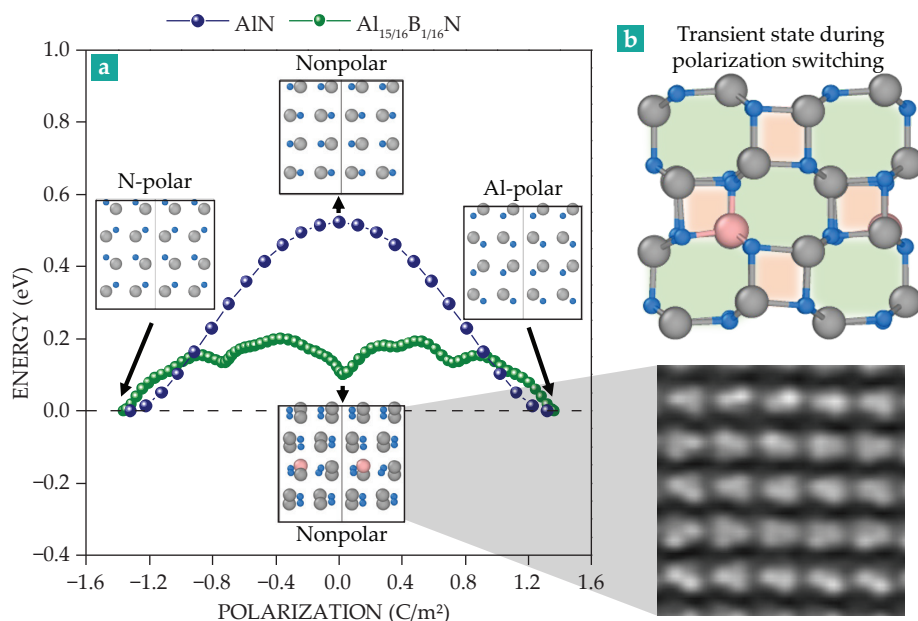


FIGURE 2. A FIRST-PRINCIPLES CALCULATION. Researchers move aluminum and nitrogen atoms in a film of aluminum nitride to determine the minimum energy pathway required to switch its polarization from N-polar to Al-polar. **(a)** Along one proposed path (blue), Al (gray) and N (light blue) atoms in each tetrahedron of a pure AlN film adopt a nonpolar, linear configuration midway. But that configuration, which has a 0.5 eV energy barrier, is never observed by transmission electron microscopy. Along an alternative path (green), the atoms switch polarization in multiple stages. **(b)** The green path's intermediate structure was confirmed (bottom) in an experiment and predicted (top) in a nearly 30-year-old simulation to include area defects in the form of four- and eight-membered rings.³ (Adapted from ref. 2.)

ential phase contrast, the microscope images the sublattices of the heavier (Al) and lighter (N) atoms at the same time. The atomic columns appear as distinct projections through the lattice.

The TEM beam also can trigger a polarization switch: As electrons scatter in the film, they ionize local Al, B, and N atoms. Electrons are ejected, and the sample becomes positively charged. When a local electric field exceeds E_c , the film's polarization switches upward (figure 1b).

Imaging the configuration of atoms during the switching process takes about seven minutes. But that time is largely spent charging the sample to the coercive field. And the TEM affords researchers the luxury of imaging continually while the charging takes place. In practice, actual ferroelectric devices flip their polarization far faster—on time scales of about a nanosecond.

Inversion through a flattened plane

When they joined the project, Maria and Dickey initially imagined that each metal

atom in a tetrahedron would break one of its N bonds. The Al or B atom would then move into the plane of the three remaining N atoms before protruding to the other side, where it would then bond with another N atom. That would be the simplest, most intuitive way to switch the polarization.

But for it to work, they realized, B atoms would be needed to flatten the tetrahedra. Like graphite, BN crystallizes in a planar hexagonal lattice, and B is energetically more likely to adopt a three-fold coordination in covalently bonded sheets than to adopt a four-fold one.

By passing through an intermediate stage in which the AlN tetrahedra flatten, the Al-N dipoles were expected to cancel and the polarization to drop to zero. In the collaboration's new work, first-principles calculations by graduate student Steven Baksa from the Dabo group bore out that imagined scenario (the blue curve in figure 2a), but only in the case of an undoped film of pure AlN. In the calculation, the 32 Al and 32 N atoms are incrementally nudged along

a proposed polarization path, during which the crystal structure diverges from a thermodynamic minimum energy state into a higher-energy, zero-polarization state. But the 0.5 eV energy barrier found by the calculation prevents that nonpolar configuration from forming.

When the researchers introduced a single B atom into the calculation, a more complicated atomic structure emerged instead—one that includes substantial local bonding and structural distortions. Both N-polar and Al-polar bonding configurations appear in the transient atomic structure, combining both upward and downward polarizations in a doubled unit cell. The B-doped AlN calculation revealed that the lowest energy path to switch the polarization is not the smooth parabolic one, but rather one with local minima (green curve in figure 2a).

Reassuringly, the collaboration's TEM image of the B-doped film (figure 2b, bottom) experimentally confirms that more complicated structure. Still more reassurance came when the researchers recognized the structure as a form of gallium nitride (figure 2b, top). It contains four- and eight-membered rings—crystallographically distinct from the parent lattice and predicted in the literature nearly 30 years ago³—in place of some of the hexagonal rings that otherwise populate the film.

The formation energy of those intermediate states—just 0.2 eV—is small enough that making them is achievable with an electric field that doesn't destroy the material. Is there an even better switching pathway that would lower the coercive field while retaining the temperature-stable polarization? The researchers don't yet know, but Trolier-McKinstry expresses hopeful enthusiasm: "We're really looking forward to finding out. For starters, we will be exploring compositional modifications that could result in lower local energies for the reversal process."

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