

A Short Tutorial on the Origin of Hysteresis in PZT

Radiant Technologies, Inc., Albuquerque, NM USA

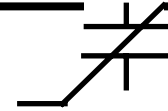
radiant@ferrodevices.com

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Why does Hysteresis Happen?

All solid materials are held together by a balance of electrical forces exerted between the atoms in material lattices. Normally, atoms in a lattice arrange themselves so that all of the electrons and protons cancel each others' electric fields.

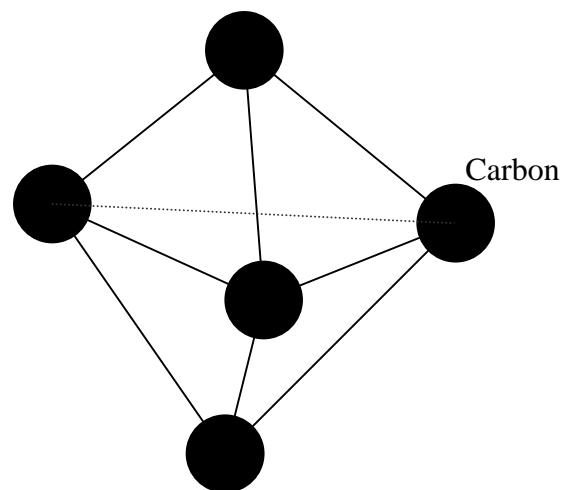
Ferroelectric materials exist with a very complex geometric structure for their lattices. This complexity gives rise to asymmetries in the lattice that prevent all of the electrical fields of the electrons and protons from canceling each other even though there are an even number of electrons and protons. From these asymmetries arise all of the useful properties of ferroelectric materials.

The Lattice and its Bonds

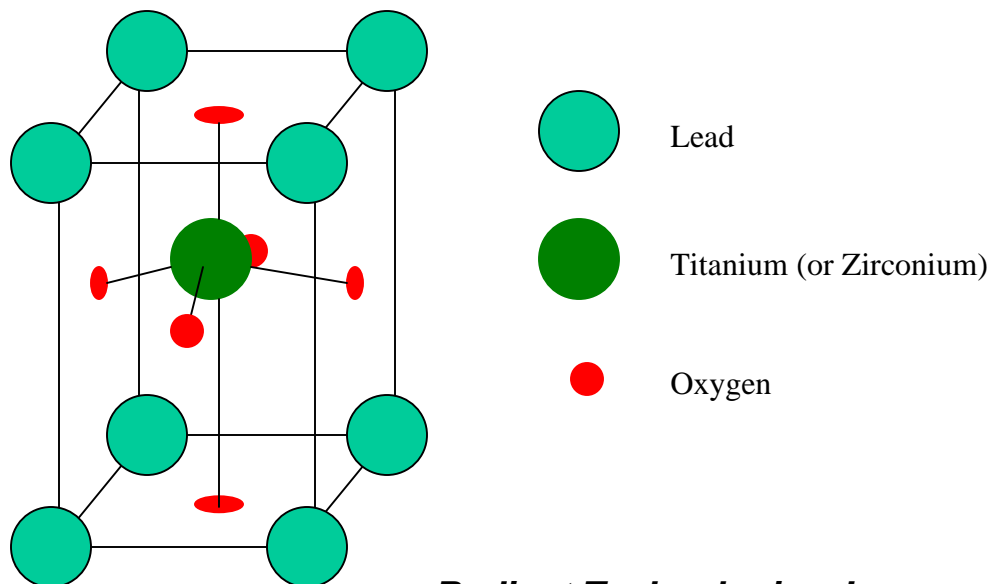
Diamond has a trihedral structure with symmetrical covalent bonds between all carbon atoms:

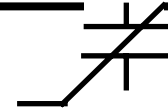
DIAMOND

Symmetrical lattice + covalent bonding means no net electric fields.



PZT has a tetragonal structure with asymmetrical, partially ionic bonds between the oxygens and the metals.

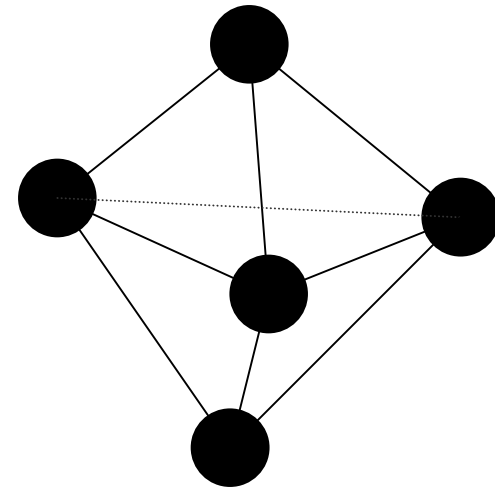




Diamond

The electrons surround each atom equally in time and space. Hence, there are no separated charges for an electric field to act on. Diamond has a low, very linear dielectric constant, ~ 5.6 .

The carbon atoms in diamond are about 1.5\AA apart along an edge. Each carbon atom occupies about 1\AA . So, as temperature goes down, there is plenty of room for the carbon atoms to move closer without bumping into each other. Diamond's electrical properties are uniform over a wide temperature range!

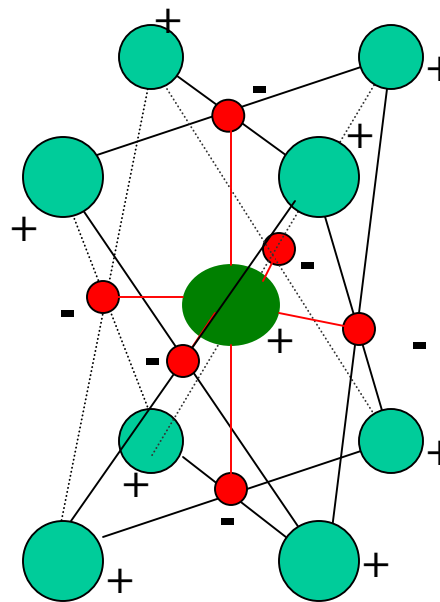


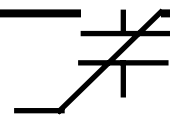
Perovskite Lattice

In the perovskite structure most ferroelectric materials have, no metals are bonded to metals. Every metal is bonded only to nearby oxygens. The bonding diagram looks like this:

The electrons stay near the red oxygens, giving every metal/oxygen pair a net electric dipole. An external electric field will repel the metals and attract the oxygens, severely distorting the lattice as it expands.

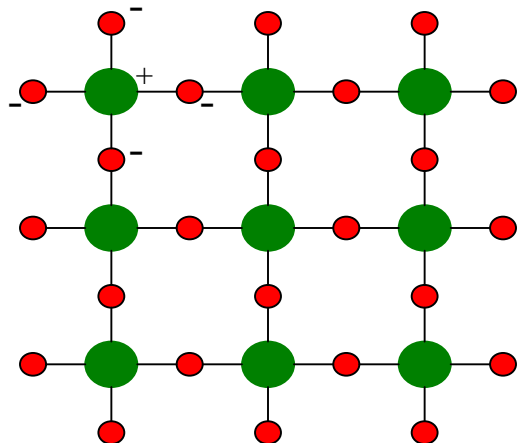
Since dielectric constant depends on physical “Displacement” (the “D” in Maxwell’s equations), perovskites can have huge dielectric constants, as high as 30,000!



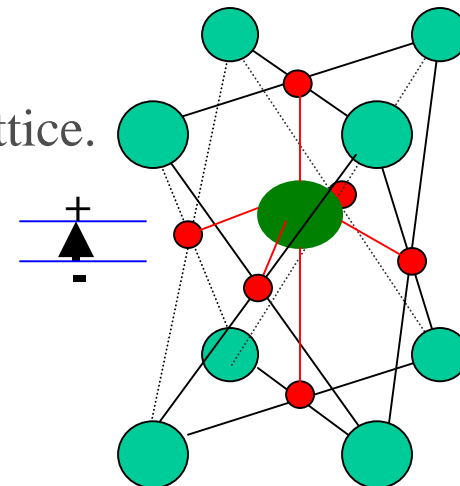
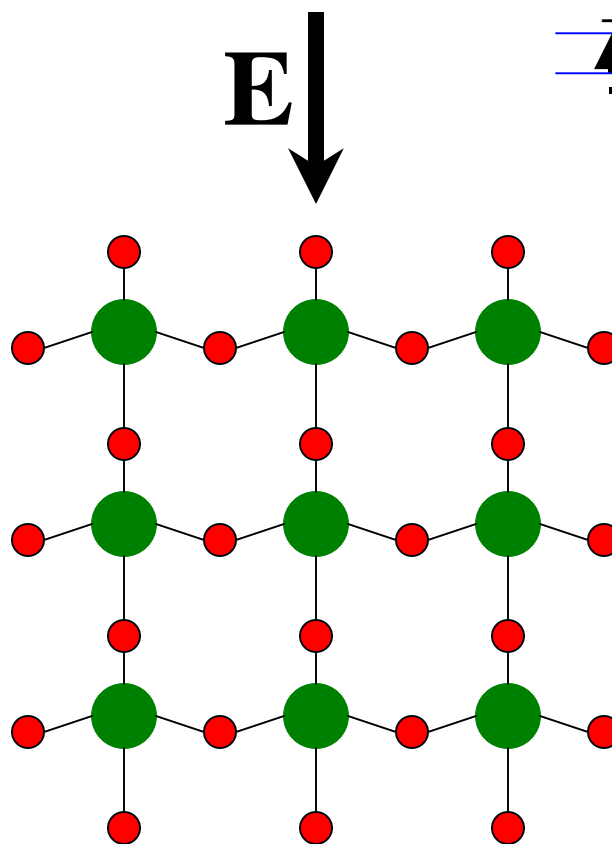


The Titanium/Oxygen Cage!

An easy way to visualize the distortion is to look at the effect of a field on the Titanium/Oxygen sub-lattice.

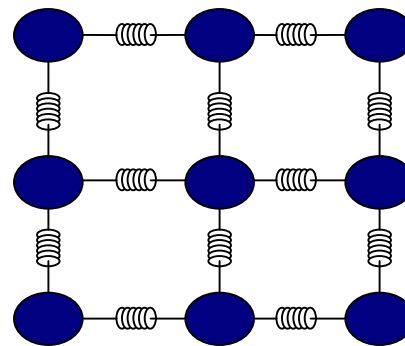
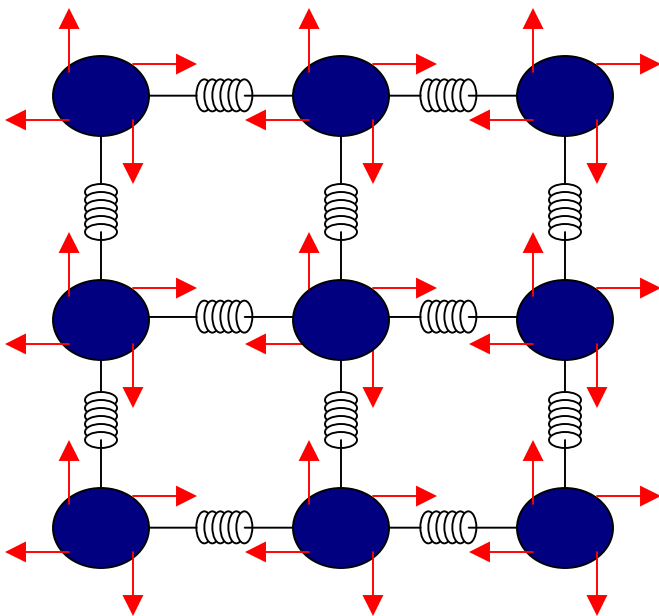


The Lead/Oxygen lattice also distorts.



Coefficient of Thermal Expansion

Solids can be treated as a network of balls and springs:



Temperature is simply the motion energy of each atom. The higher the temperature, the faster they move, the harder they bounce off each other, and the further apart they force each other to stay. Hence, physical size of solids changes with temperature. The change in dimensions vs the change in temperature is the **Coefficient of Thermal Expansion!**

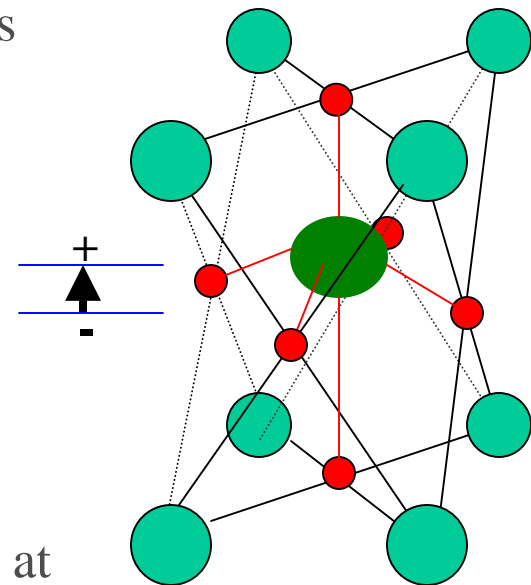
The CTE of PZT is ~15 times that of Diamond.

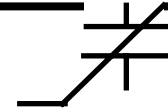
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Remanent Polarization

PZT has a 4\AA lattice constant, but many more atoms are squeezed into the that volume than with diamond! As the temperature drops and the lattice shrinks, eventually, there is not enough room for all the atoms in the symmetrical format. So, the lattice distorts to squeeze the atoms closer together. A simple model, called the “rattling titanium” model, is that the the body-centered atom slides up about 0.05\AA so it is no longer co-planar with the oxygens.

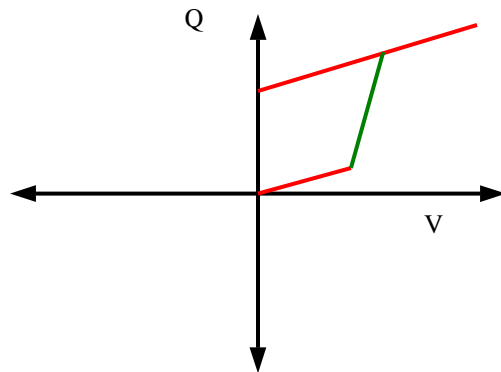
Since the titanium’s electrons stay mostly around the oxygens, a net vertical dipole is created at room temperature.





Finally: Hysteresis!

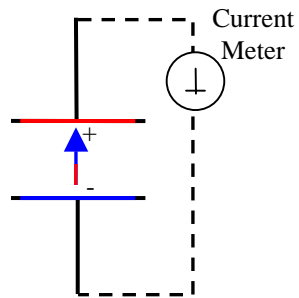
In many materials called “electrets”, the lattice is rigid and the internal dipoles are fixed relative to the lattice, never to switch. Ferroelectric materials, on the other hand, have just the right amount of softness so external forces like an electric field can make the charged atoms shift position to line up with the voltage but the right amount of rigidity so the resultant dipoles stay lined up when the force is removed at zero volts.



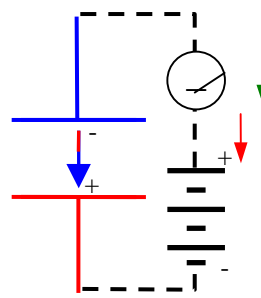
The next page shows how dipoles make this “half” hysteresis loop.

The Electrical Measure of Hysteresis!

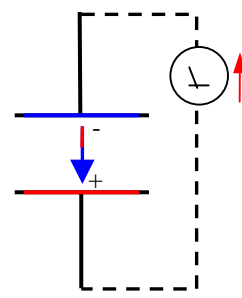
- Negative Charge
- Positive Charge



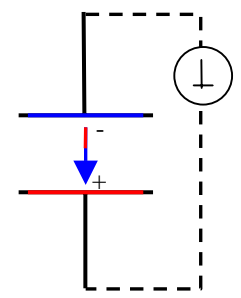
(a)
Dipole starting at zero volts.



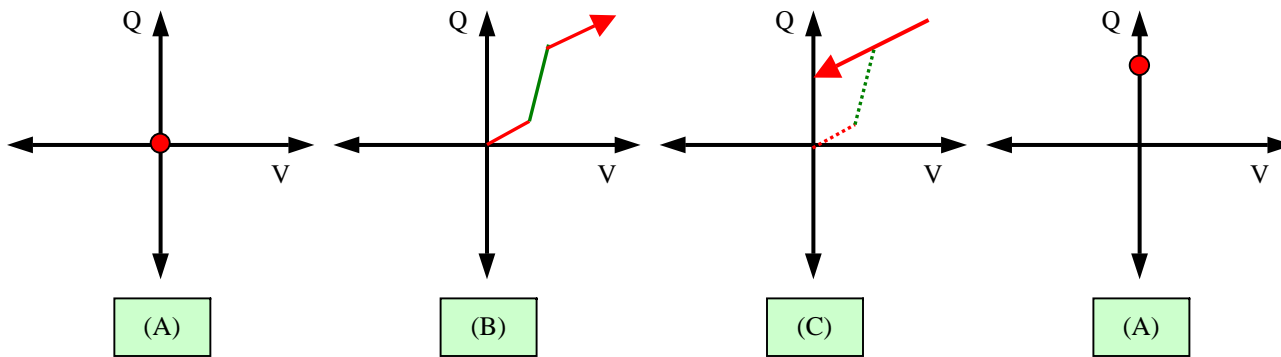
(b)
Apply voltage and charge capacitor in opposite direction as dipole. Dielectric and remanent charge both move.



(c)
Discharge capacitor.

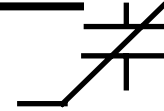


(d)
Dipole at zero volts again and in the opposite direction.

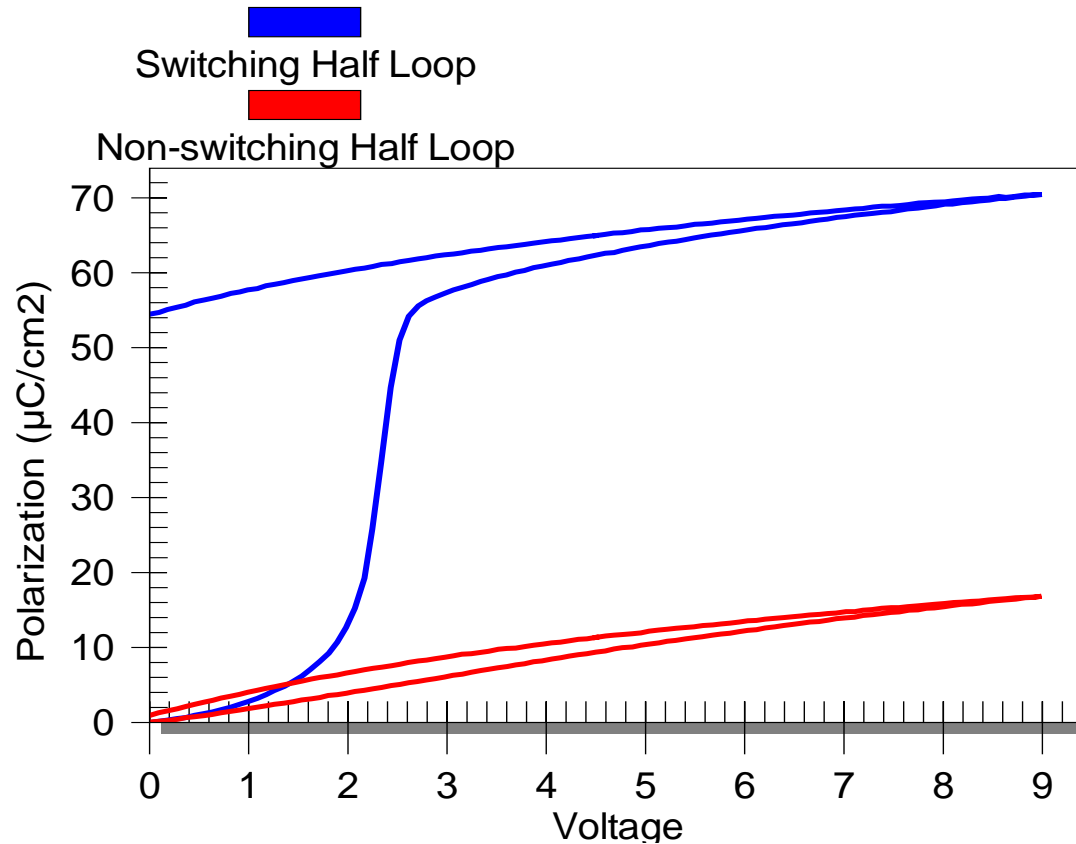


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Memory



Half Loops in a PZT Capacitor [Radiant Type AB White]

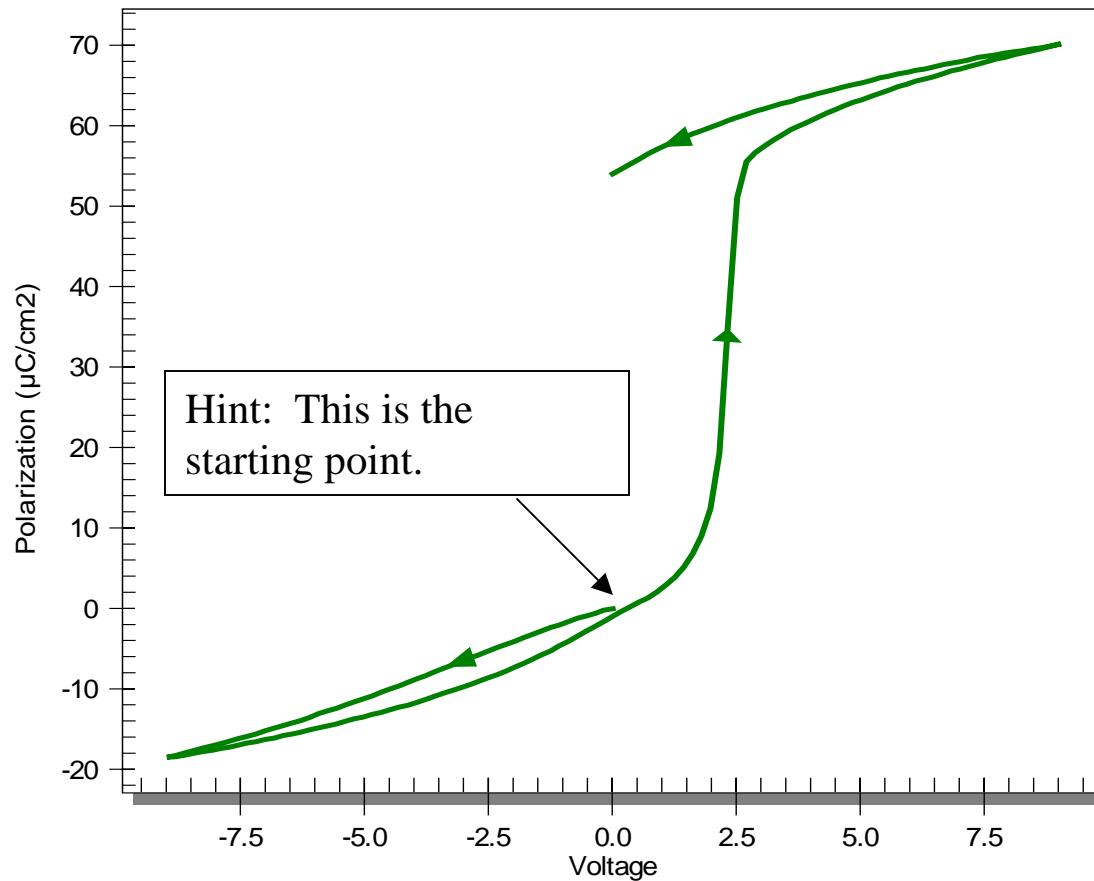


The ferroelectric capacitor will give a “little bit” of charge or a “lot” of charge depending on the direction of the applied voltage and the direction of the dipoles. This property is used in modern Ferroelectric RAM ICs to make high-speed non-volatile memory chips.

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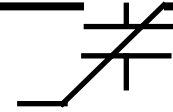
Mysteries of Memory

Packaged PZT Capacitor
[Radiant Type AB White]



What is this waveform? It happens millions of times a second to individual data bits in a magnetic disk drive when new data is written to the disk. Disk drives depend on magnetic hysteresis to store data.

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Conclusion: Hysteresis!

Electrical hysteresis arises in ferroelectric materials much like magnetic hysteresis in magnetite, a material with which many more people are familiar. Materials engineers, tinkering with composition and process, can now fabricate new ceramic materials with strong ferroelectric properties and usefulness.