A Short Tutorial on the Origin of Hysteresis in PZT

Radiant Technologies, Inc., Albuquerque, NM USA

radiant@ferrodevices.com

Rev D

April 3, 2013

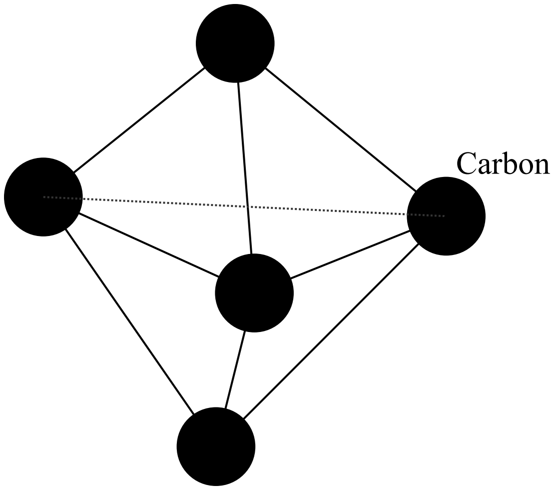
Why does Hysteresis Happen?

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 lattice. 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

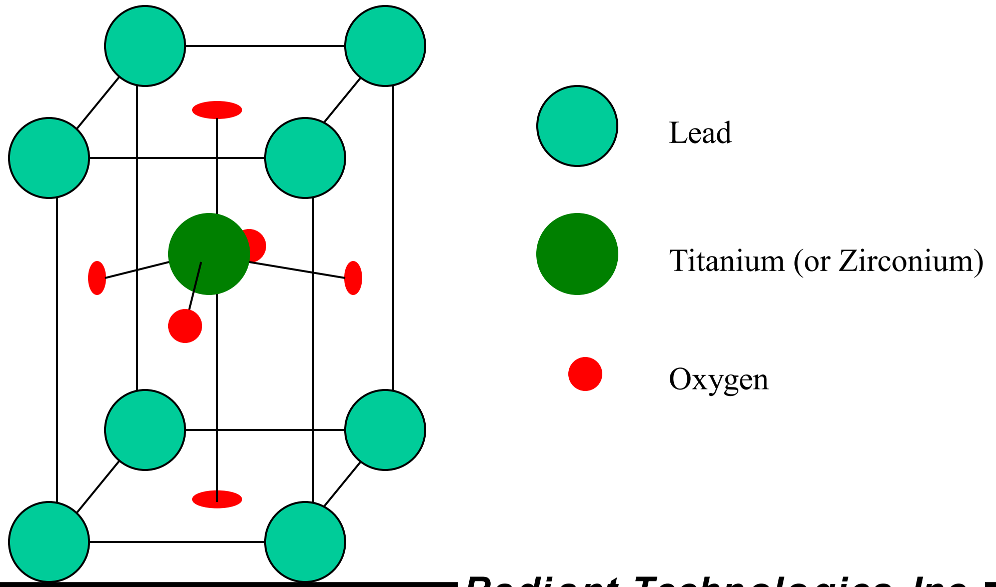
Diamond has a trihedral structure with symmetrical covalent bonds between all carbon atoms:



DIAMOND

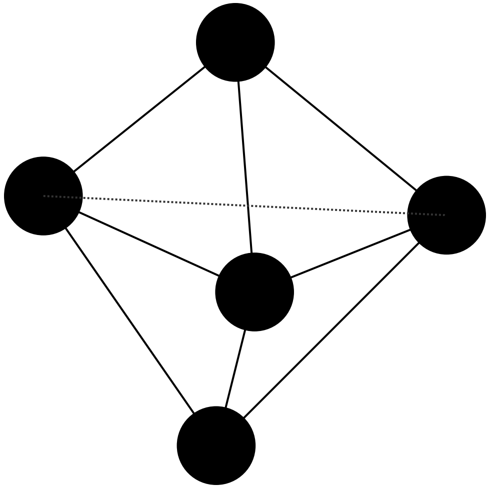
Symmetrical lattice + covalent bonding means no net electric fields.

PZT has an asymmetrical structure with partially ionic bonds between the oxygen and metal atoms.



Diamond

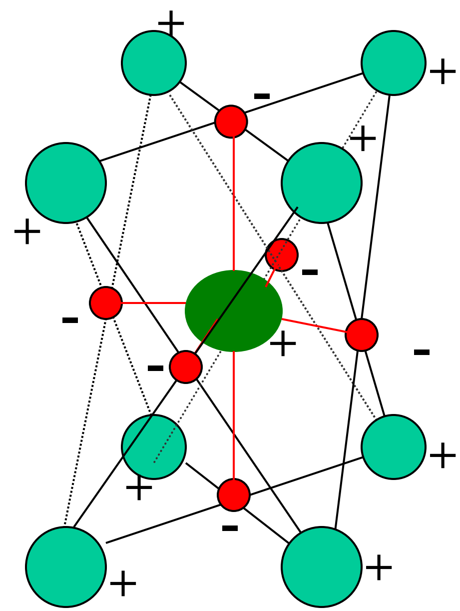
The electrons surround each atom equally in time and space. Hence, there are no separated charges for an electric field to act on. Diamond has a low, very linear dielectric constant, ~5.6.



The carbon atoms in diamond are about 1.5Å apart along an edge. Each carbon atom occupies about 1Å. 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 of many ferroelectric materials, no metals are bonded to metals. Every metal atom is bonded only to nearby oxygen atoms. The bonding diagram looks like this:

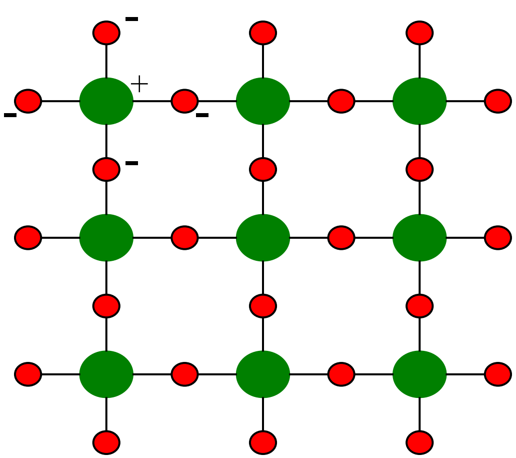


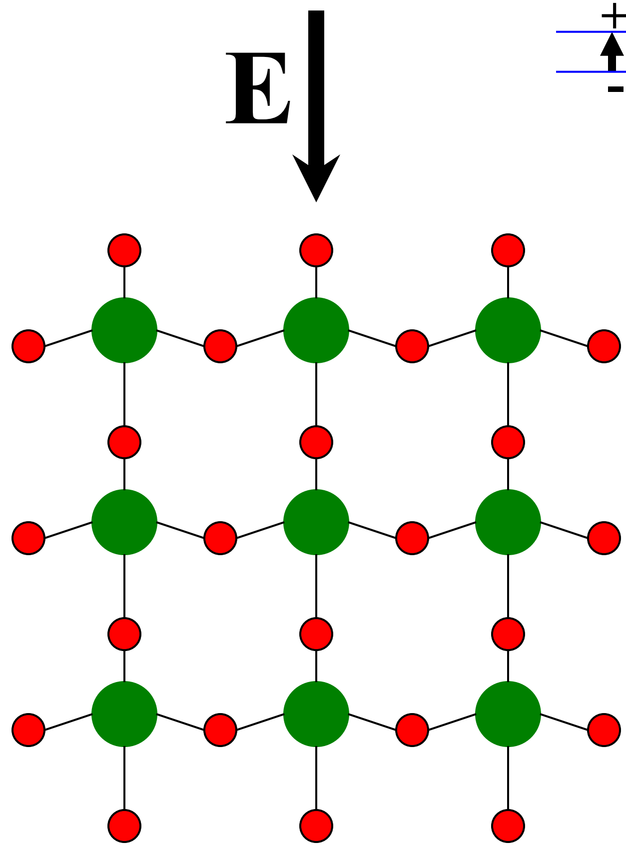
The electrons stay near the red oxygen atoms, giving every metal/oxygen pair a net electric dipole. An external electric field will repel one half of the pair and attract the other half, severely distorting the lattice.

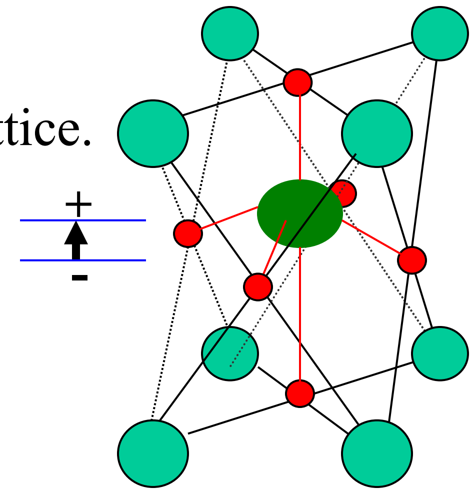
Since dielectric constant depends on physical "Displacement" (the "D" in Maxwell's equations), perovskites can have huge dielectric constants, as high as 30,000!

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.



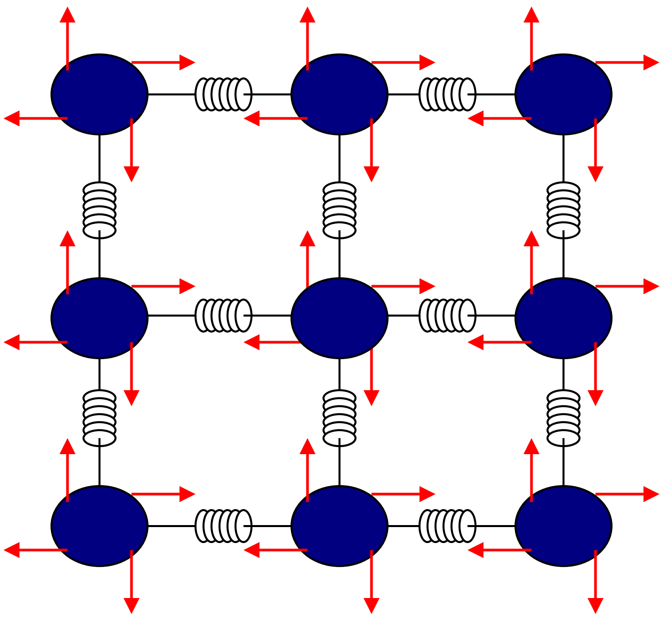




The Lead/Oxygen lattice also distorts.

Coefficient of Thermal Expansion

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



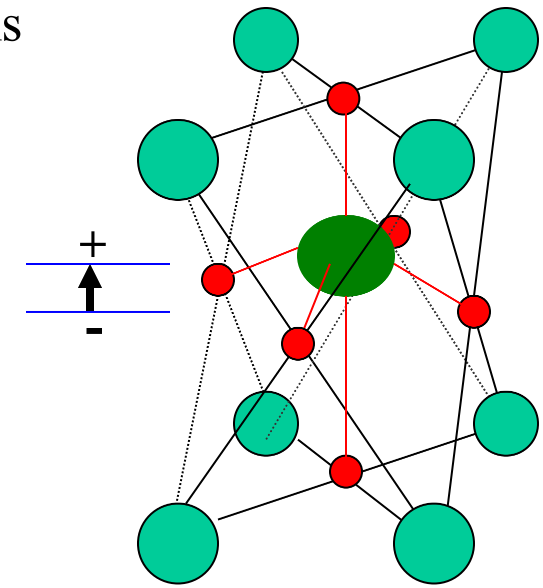
Temperature is simply the motion energy of each atom. The higher the temperature, the faster each atom moves, the harder they bounce off each other, and the further apart they force each other to stay on average. Hence, the physical size of solids changes with temperature.

The change in dimensions vs the change in temperature is called the Coefficient of Thermal Expansion!

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

Remanent Polarization

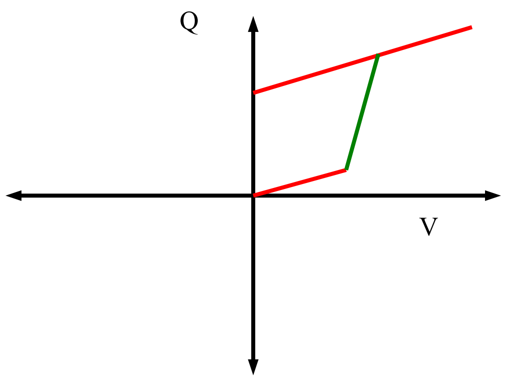
PZT has a 4Å lattice constant, but many more atoms are squeezed into the that volume than with diamond! As the temperature drops and the lattice shrinks, eventually, there is not enough room for all the atoms in a symmetrical format. So, the lattice distorts to squeeze the atoms closer together. A simple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



Since the titanium's electrons stay mostly around the oxygen atoms , a net vertical dipole is created for each unit cell at room temperature.

Finally: Hysteresis!

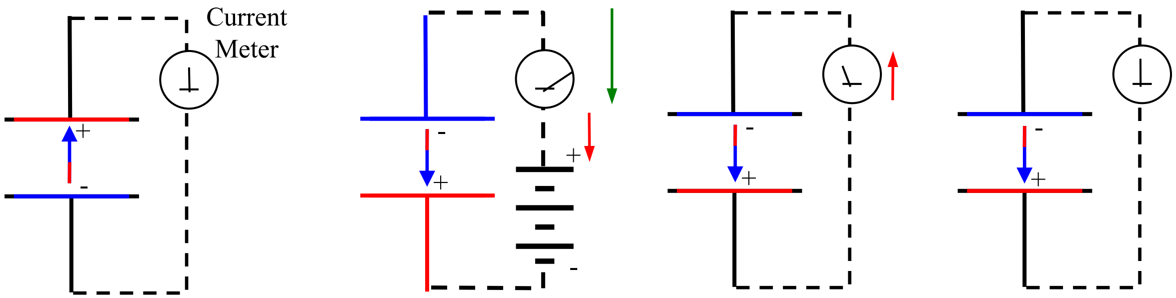
In many materials called "electrets", the lattice is rigid and the internal dipoles are fixed relative to the lattice, never to switch. Ferroelectric materials, on the other hand, have just the right amount of softness so external forces like an electric field can make the charged atoms shift position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



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

The Electrical Measure of Hysteresis!

— Negative Charge
— Positive Charge

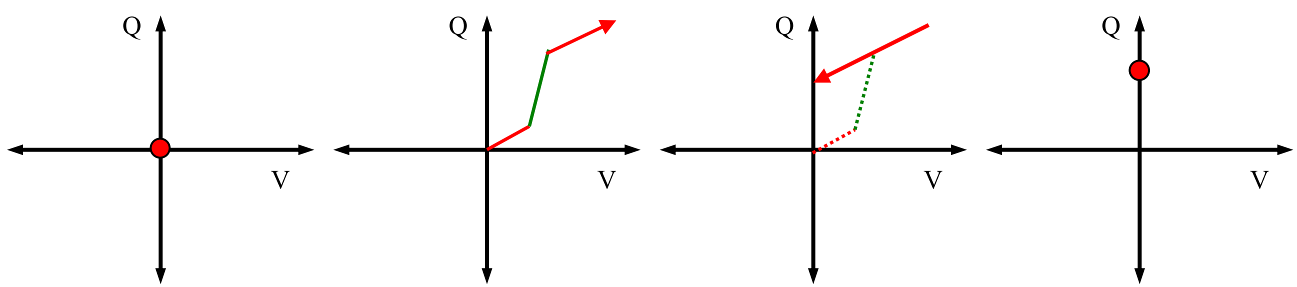


(a)
Dipole starting at zero volts.

(b)
Apply voltage and charge capacitor in opposite direction from dipole. First the dielectric and then remanent charge move.

(c)
Discharge the dielectric charge from the capacitor. The remanent charge remains.

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



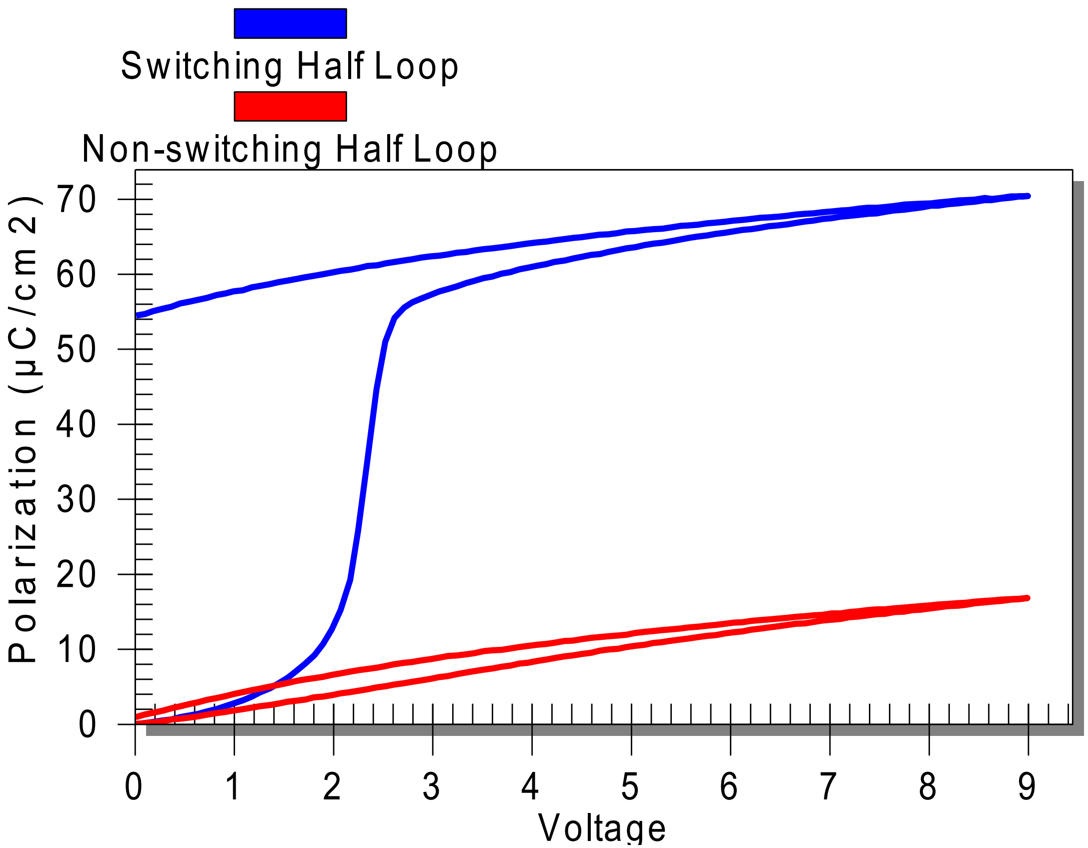
(A) (B) (C) (A)

Radiant Technologies, Inc.

Memory

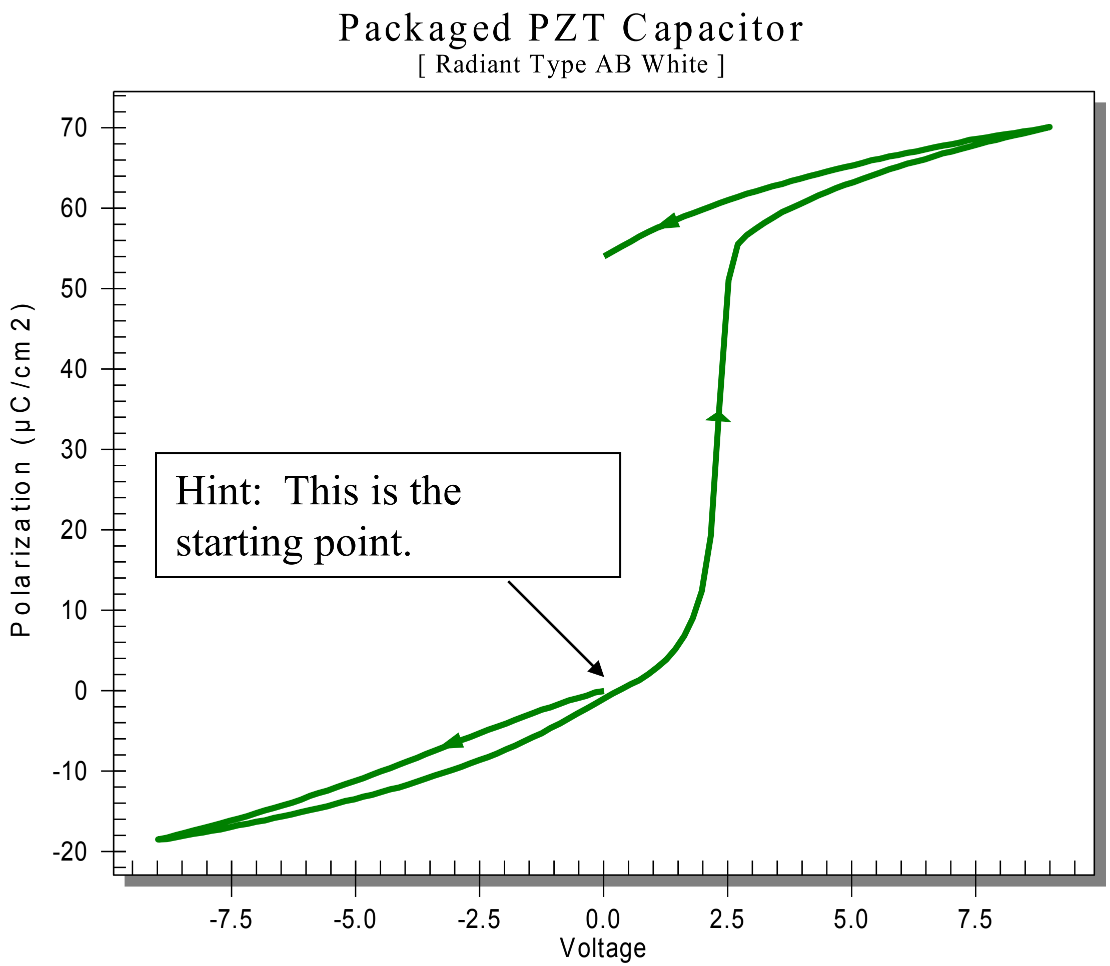
Half Loops in a PZT Capacitor

[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 starting direction of the dipoles. This property is used in Ferroelectric RAM ICs to make high-speed non-volatile memory chips.

Mysteries of Memory



What else looks like 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.

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 fabricate many different ceramic thin-film materials with useful ferroelectric properties.