

## **Ferroelectricity in perovskite oxides: Origin and Application**

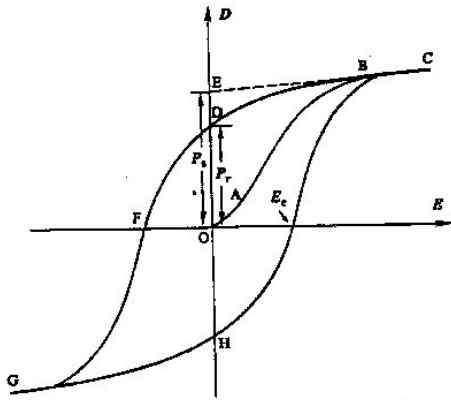
Change is inevitable for the entire human species. There is a drive of some sort that pushes us onward and toward the next step of evolution. History has many instances of the evolution made through the various years, century or millennia. History tells us that the evolution of man is measured by the sophistication of his work. This sophistication of his technique shows how man control and master its environment. It is this very inevitable drive that rushed us to the era of high technology devices, just to mention two instances: computers went from humongous to thin and very portable, gramophone is now obsolete and music is brought to you nowadays to your ear canal by the earphones plugged to a “jukebox” that can fit into your pocket.

What is happening behind the scene though is another story, very interesting, that we are going to discuss in this paper. Taking you through the paper, as the title suggests, we are going to discuss first about ferroelectricity: mainly the idea behind it and the reason it is exhibited in some materials, particularly the materials that are called “perovskite”, and some instances of its application.

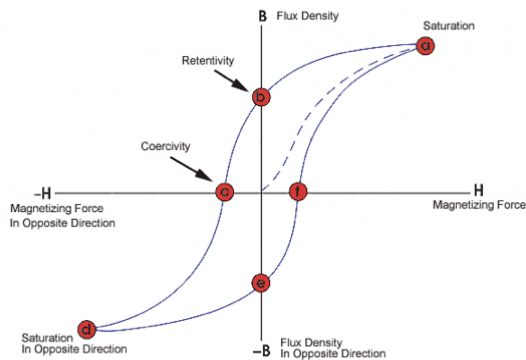
Let us go ahead and find out what is the idea behind ferroelectricity.

In 1921, this phenomenon that we come now to call ferroelectricity was discovered in Rochelle salts, a few example of those are:  $\text{NaK}(\text{C}_4\text{H}_4\text{O}_6) \cdot 4\text{H}_2\text{O}$ ,  $\text{NaK}(\text{C}_4\text{H}_2\text{D}_2\text{O}_6) \cdot 4\text{D}_2\text{O}$ , then it has been discovered such as perovskite around the 1942. Our peaked interest in this material will be justified and explained in the later paragraphs of this paper. Let us clear up a fact about the name “Ferroelctricity.” This is a misnomer in the sense that it is not linked to iron or ferrum. The reason for this nomenclature is due to its analogy in magnetic theory, namely the ferromagnetism property. A little reminder that the reaction of materials to magnetic field differs: there are those materials whose magnetic moments are oriented along the direction of an applied magnetic field called “diamagnets” and there are those materials whose magnetic moments are oriented in the opposite direction of the applied magnetic field called “paramagnets.” Finally there is what is called “ferromagnet”, which are material that exhibit permanent magnetic moment after an applied magnetic field.

A ferroelectric material then exhibits an electric dipole moment even in the absence of an external field. Just like its magnetic parallel it has the hysteresis curve:



<http://www.rci.rutgers.edu/~ecerg/projects/ferroelectric.html>



<http://www.ndt-ed.org/EducationResources/CommunityCollege/MagParticle/Physics/HysteresisLoop.htm>

Just like in the magnetic theory the hysteresis curve in ferroelectric describes the polarization state of a ferroelectric material. It is good to point out that this property tends to disappear for ferroelectric materials above a temperature that is called transition temperature ( $T_c$ ), some calls this the Curie point, past which the material becomes paraelectric, meaning the dielectric constant decrease rapidly as the temperature increases.

Among the materials exhibiting ferroelectricity we have the group of crystals called perovskites for instance: Barium titanate ( $BaTiO_3$ ), Lead titanate ( $PbTiO_3$ ). Those materials have Curie point going from  $T_c = 223K$  to  $T_c = 763K$ . Those materials are called perovskite because they have the same crystal structure as a  $CaTiO_3$  just like in the crystal structure of fig3 below.

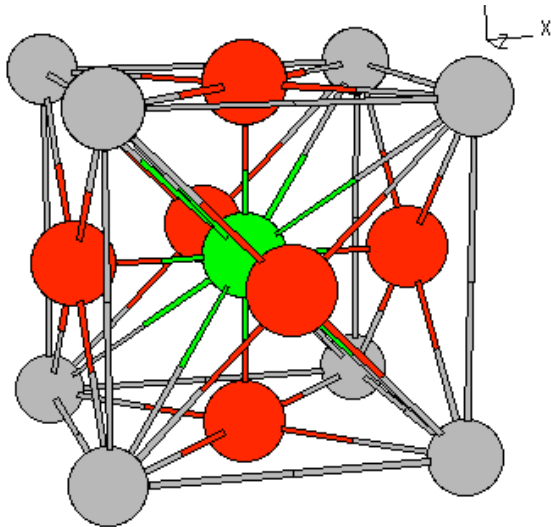


fig 3 ([http://cst-www.nrl.navy.mil/lattice/struk.picts/e2\\_1.s.png](http://cst-www.nrl.navy.mil/lattice/struk.picts/e2_1.s.png))

The central atom is the Titanium atom or the B-atom, the 6 red atoms surrounding it are the oxygen atoms with the 8 atoms remaining atoms being in general called an "A" atom where it can be Calcium, Barium or Lead.

So some crystals of this configuration exhibit this property. What then is the responsible for this polarization in the ferroelectric perovskite oxides? What is believed is that: "The displacement of the positive and negative ions results in the polarization that characterizes ferroelectric materials."<sup>1</sup> It can easily be seen that a displacement of the central atom in the structure creates an unbalance that result in a net polarization.

Few more interesting facts are that both the Lead titanate as well as the Barium titanate have the same crystal lattice structure but prove to differ in various properties for example: phase transitions, BaTiO<sub>3</sub> has cubic to tetragonal, tetragonal to orthorhombic and orthorhombic to rhombohedral whereas PbTiO<sub>3</sub> has only the cubic-tetragonal phase transition.<sup>2</sup> These differences incite us to look more into the unit cell and find out what actually, besides the central atom displacement, is at the origin of the ferroelectricity. What differ both materials are the A-atoms namely: Ba and Pb. We can intuitively think that if ferroelectricity were to be a property of both materials, it can only arise from the interaction between the other two common elements of both materials. The comparative study of BaTiO<sub>3</sub> and PbTiO<sub>3</sub> verified our intuition. "Computation without assumptions about bonding, ionicity or shape of the charge"<sup>2</sup> were used and led to the conclusion that "for ferroelectrics in general, hybridization between the B atom (cation) and O is essential for ferroelectric transition."<sup>2</sup>

Now that we know about ferroelectricity, let us discuss about the way to take advantage of this property and make good use of it. Let us first stress the fact that by applying an electric field we can change the direction of the polarization.

At this point we are ready to explain our particular interest in perovskite oxides. First because of its high dielectric constant given by

$$\epsilon = \frac{[1 + \left(\frac{8\pi}{3}\right) \sum_i (N_i \times \alpha_i)]}{[1 - \left(\frac{4\pi}{3}\right) \sum_i (N_i \times \alpha_i)]}, \text{ where } N_i \text{ is the number of ions } i \text{ per unit volume and } \alpha_i \text{ is}$$

the polarizability of an ion of type  $i^3$ , materials like Barium titanate make very high capacitance capacitor. Because of its tunable polarization people has looked into having what is called a Non Volatile Ferroelectric Random Access Memories or short NVFRAMs, where can use the polarization as the binary if it is one way 1 or 0 if it is the other way<sup>1</sup>. Along with ferroelectricity we have properties like piezoelectricity and pyroelectricity. The former is the electrical response of the material to mechanical stress and vice versa, whereas the latter is about the polarization due to small change in temperature<sup>4</sup>. Those properties can be exploited to use the material as sensor or as other devices.

### **Bibliography:**

- 1- **The physics of ferroelectrics memories**, Orlando Auciello, James Scott and Ramamoorthy Ramesh, Physics Today, July 1998
- 2- **Origin of ferroelectricity in perovskite oxides**, R.E. Cohen, Nature Vol 358, 9 July 1992.
- 3- **Introduction to Solid State Physics** 3<sup>rd</sup> edition, Charles Kittel, John Wiley, page 407

4- <http://www.rci.rutgers.edu/~ecerg/projects/ferroelectric.html>