Phase Transition and hysteresis loops in ferroelectric materials

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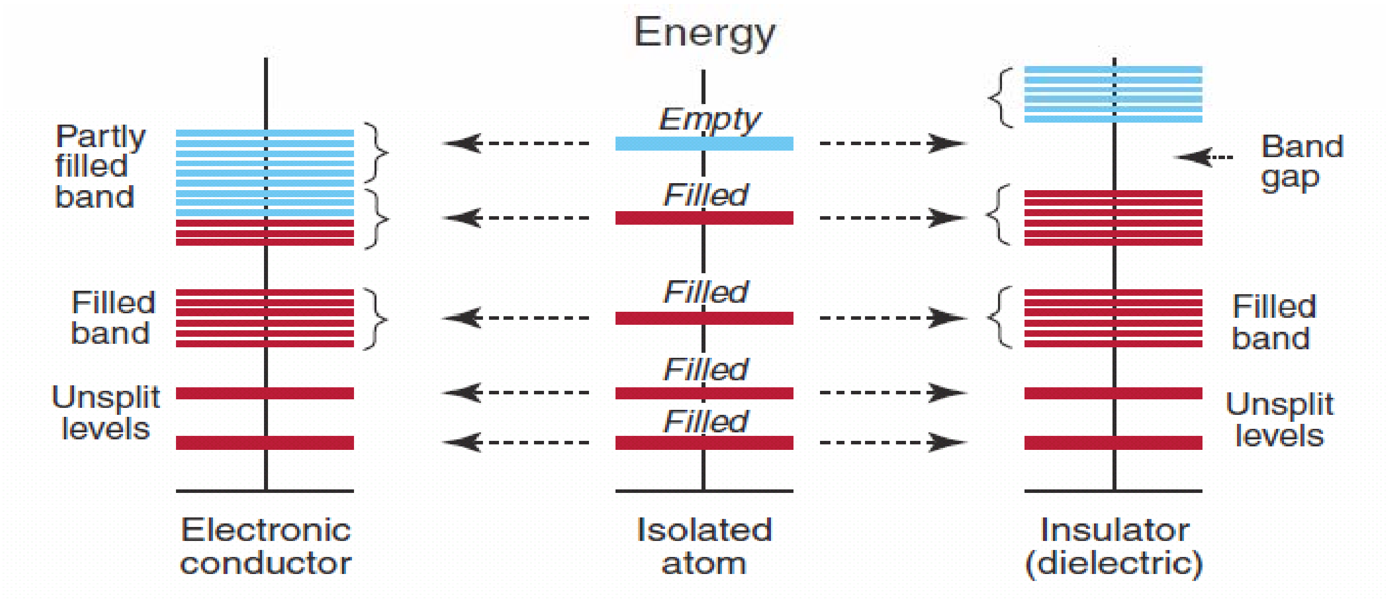
24-09-2010

- **Outlines**

- Insulators
- Functional insulators
- Ferroelectrics
- Phase transition in $BaTiO_3$
- Ferroelectricity in $BaTiO_3$
- Sawyer Tower Circuit for KNO_3
- Observation of ferroelectric hysteresis loops of KNO_3 thin films
- Future plan

Insulators

- Whether the material is a conductor or an insulator depends on how full the bands are, and whether or not they overlap.



An insulator is a material having conductivity in the range of 10^{-10} to 10^{-16} $\Omega^{-1}m^{-1}$

Functional Insulators

- **Dielectrics**
- **Piezo-electrics**
- **Ferroelectrics**

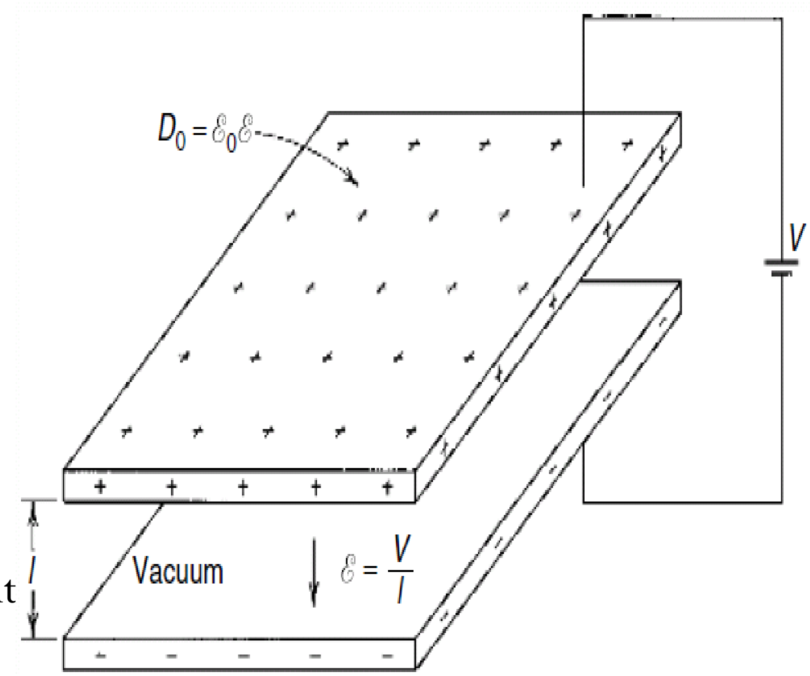
A dielectric material is any material that support charge without conducting it to a significant degree or any electrical insulator is also called a dielectric.

In vacuum

$$\mathscr{E} = V/l$$

But the magnitude of charge per unit area on either plate is called 'electric displacement'

$$\mathbf{D}_0 = \varepsilon_0 \mathscr{E}$$



Here $\mathbf{D}_0$ (C/m^2) is called electric displacement and also called surface charge density on the plate in vacuum

Dielectrics (continued)

- The surface charge density can be related to capacitance of a parallel plate capacitor in vacuum as follows:

$$C_0 = q/V$$

But $q = D_0 A$

Then $C_0 = \varepsilon_0 \frac{A}{l}$

Here C_0 = capacitance in vacuum

ε_0 = permitivity of free space

A= Area of the plates

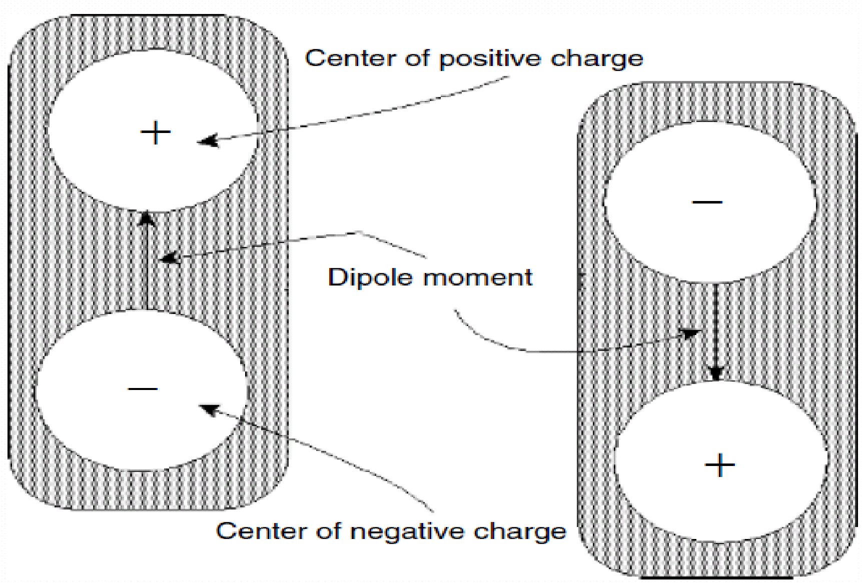
ℓ = distance between the plates

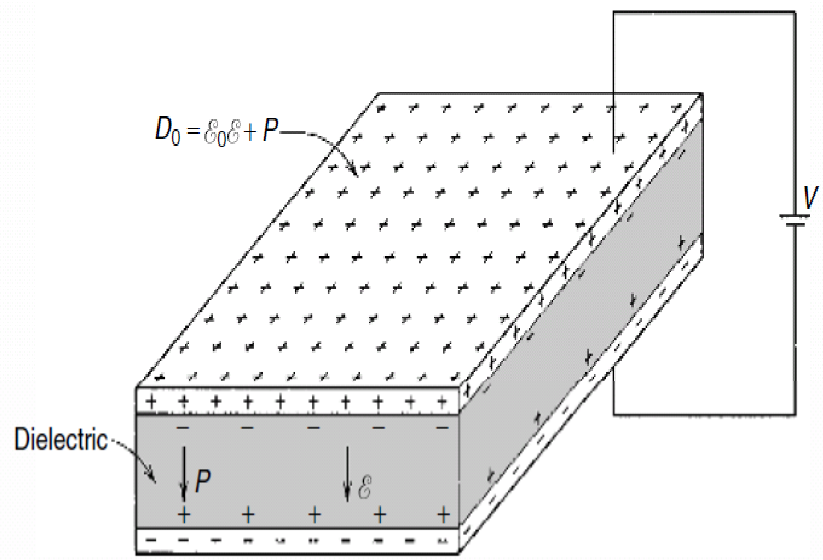
q = charge on each plate

V = P.D between the plates

Dielectrics (continued)

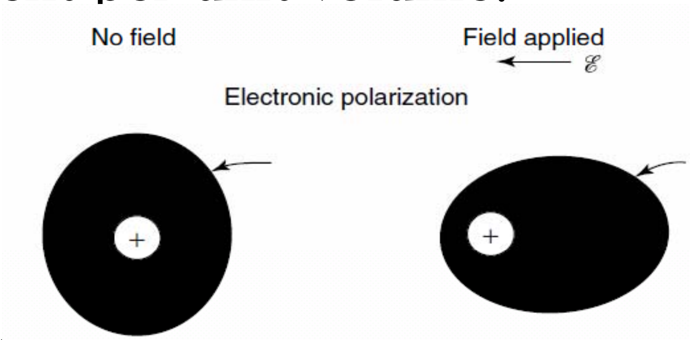
In the presence of 'Dielectric material'
A displacement of charge within the material is created through a progressive orientation of permanent or induced dipoles.





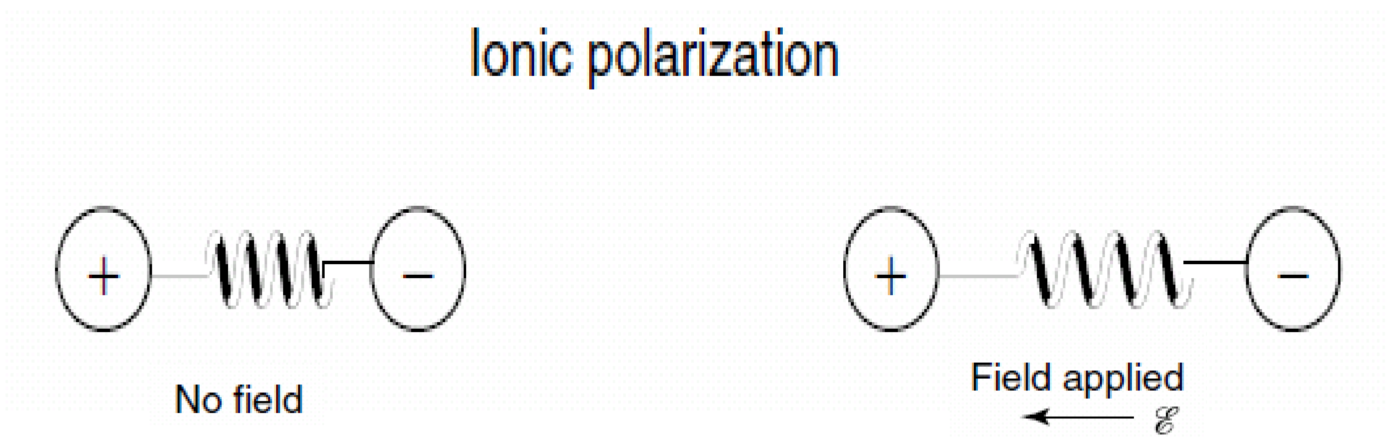
Polarization

- The interaction between permanent or induced electric dipoles with an applied electric field is called polarization, which is the induced dipole moment per unit volume.
- **Electronic Polarization**
- It occurs due to centre of the electron cloud around a nucleus is displaced under an applied electric field. It gives rise to net dipole moment per unit volume.



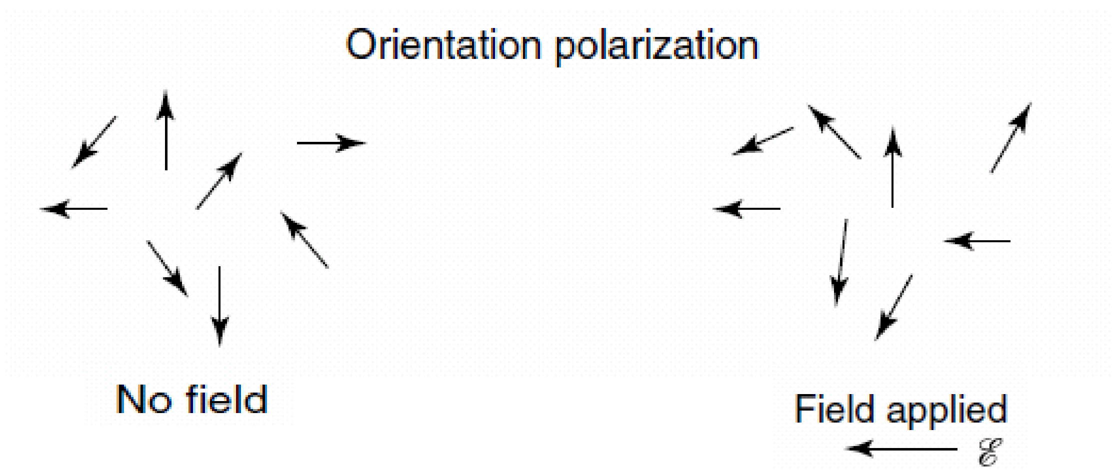
Ionic Polarization

- It occurs in ionic materials because an applied field acts to displace cations in the direction of the applied field while displacing anions in a direction opposite to applied field. It gives rise to dipole moment per formula unit.



Orietational Polarization

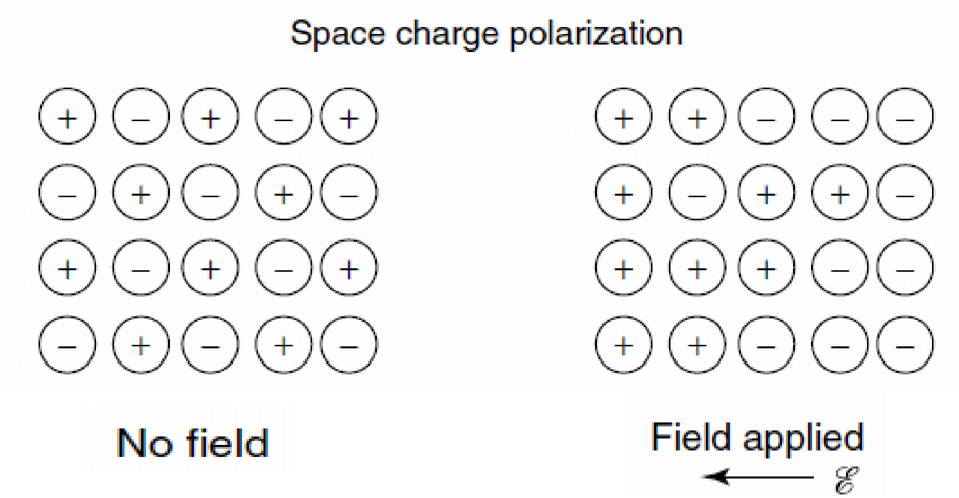
- It is temperature dependent polarization. It occurs in materials composed of molecules that have permanent electric dipole moments. The permanent dipoles tend to become aligned with the applied electric field, but entropy and thermal effects tend to counter this alignment.



e.g Liquid and gases where molecules are free to rotate

Space-Charge Polarization

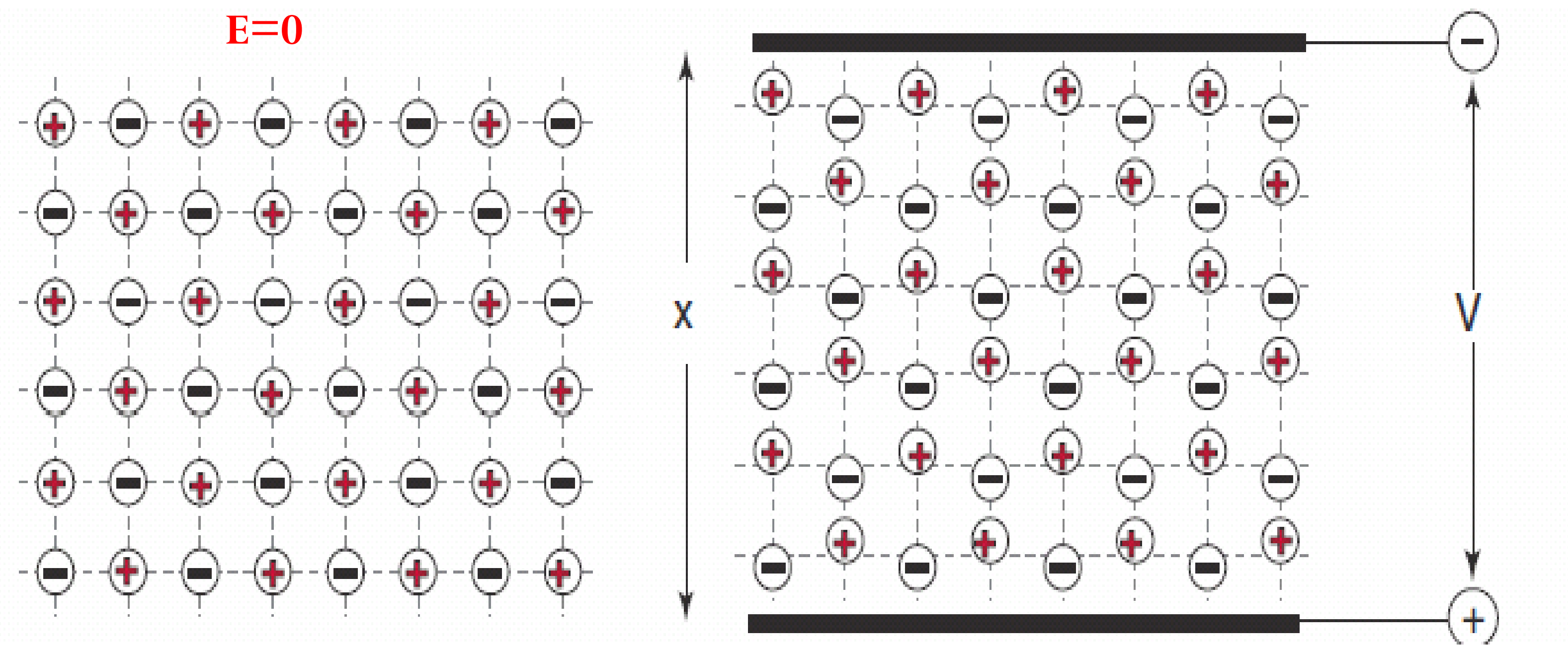
- It results from the accumulation of charge at structural interfaces in heterogeneous materials. Such polarization occurs when one of the phases has a much higher resistivity than the other, it is found in a variety of ceramic materials.



Note:

- ***D*** *is connected with the free charge only. The lines of* ***D*** *begin and end on free charges.* ***D*** *is constant throughout the capacitor.*
- ***P*** *is connected with polarization charge only.* ***P*** *is zero except inside the dielectric.*
- ***E*** *is connected with all charges.*
- *In isotropic media* ***P*** *and* ***E*** *are in the same direction.*
- ***E*** *is reduced inside the dielectric.*
- *The units of* ***P*** *and* ***D*** *are* $\mathbf{C/m^2}$

What happens to electrons in “Dielectrics” when electric field is applied?

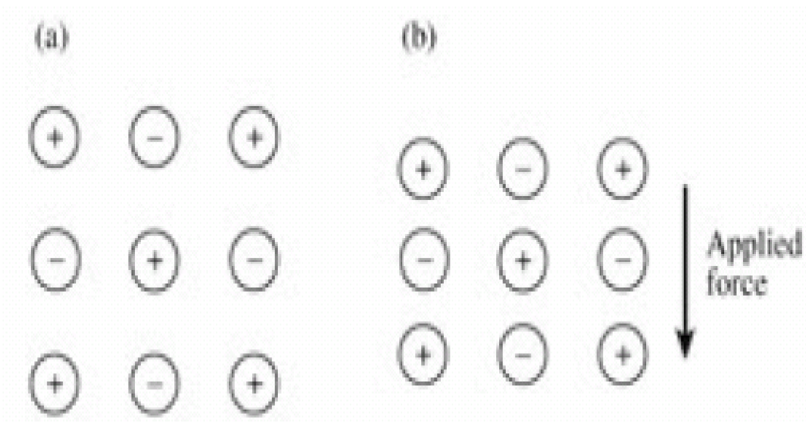


Piezo-electric materials

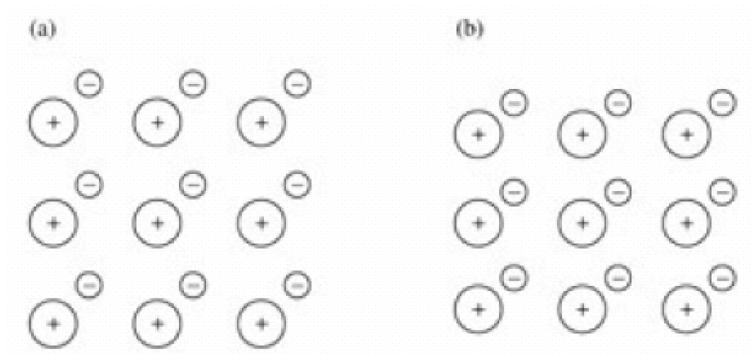
- Word------Quartz-----written on the face of watch----means
- **Time steps are set by the oscillations of a piezo-electric quartz crystal.**
- **Piezo-electric effect**

  A mechanical strain will produce dielectric polarization and, conversely, an applied electric field will cause mechanical strain.
- **Crystals having lack of centre of symmetry exhibit this effect.**

Piezo-electric effect in symmetric and non-symmetric cubic crystals



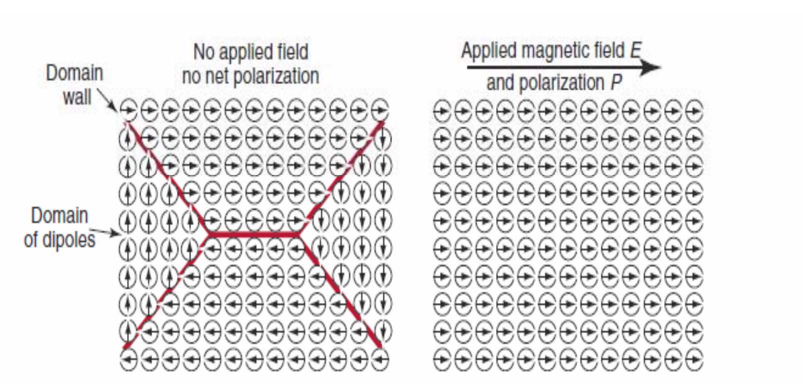
Symmetric cubic structure



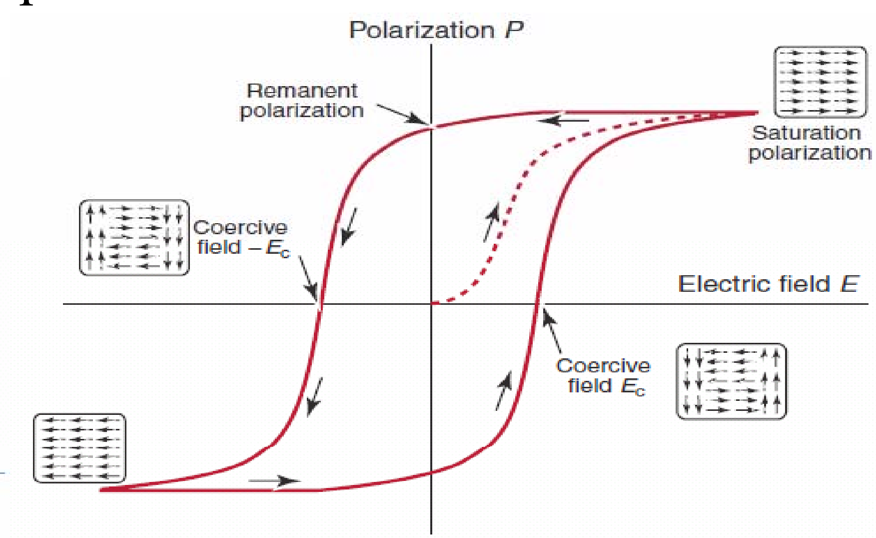
Non-symmetric cubic structure

Ferroelectricity

- Spontaneous alignment of electric dipoles by their mutual interaction in the absence of an applied electric field.
- **Source of ferroelectricity**
- It arises from the fact that the local field increases in proportion to the polarization. Thus, ferroelectric materials must possess permanent dipoles.



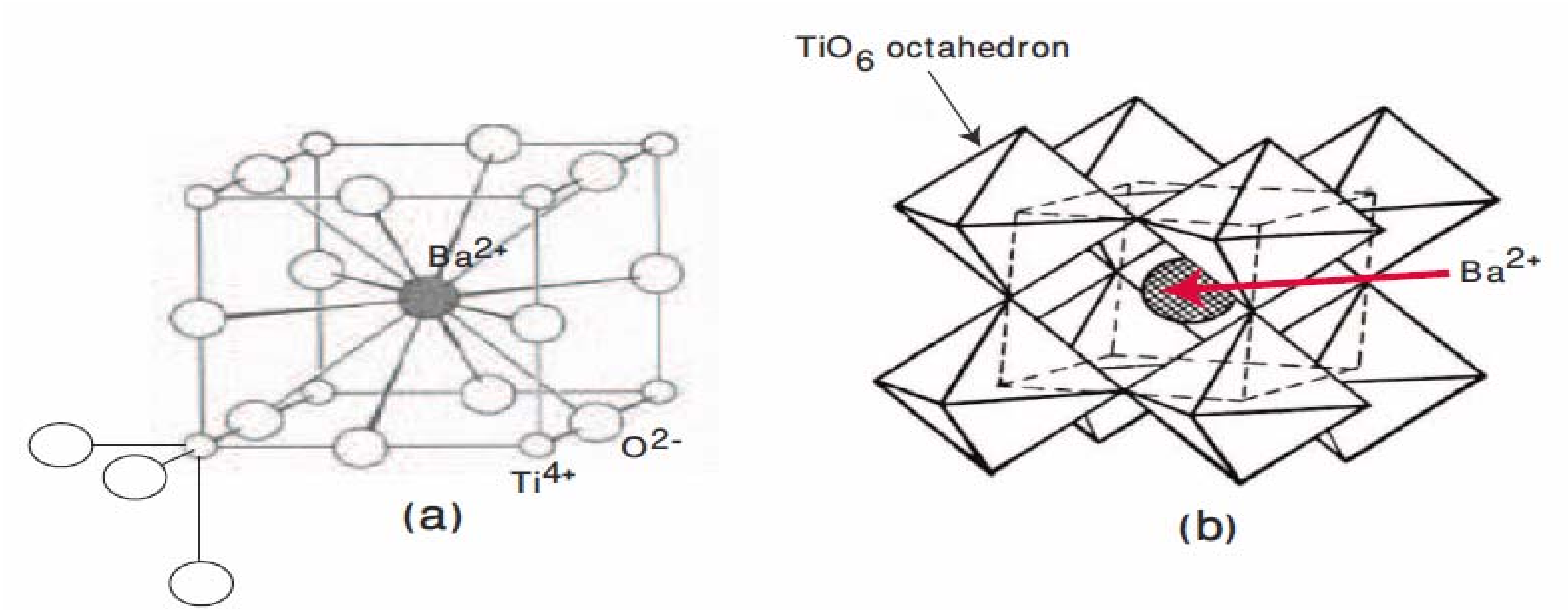
Ferro-electric domains arrange themselves so that their dipole moments cancel. In an electric field E they align, giving the crystal a net dipole moment, which can be large.



Why Ferroelectric Materials?

- Ferroelectric materials are special case of piezo-electric behavior. They too have an unsymmetric structure, but have the special ability to switch asymmetry. So to be ferroelectric, a material must possess a spontaneous dipole moment that can be switched in an electric field.
- Ferroelectric materials are non-centrosymmetric i-e central atom must be in a non-equilibrium position.
- Normal materials with symmetric charge distribution have dielectric constant in the range of 2-20 but ferroelectric materials have 20,000, this allows their use to make super-capacitors that can store 1000 times more energy than conventional capacitors and can be competed with batteries for energy storage.
- **Examples**
- **$BaTiO_3$, KNO_3, $PbTiO_3$,PZT and $BiFeO_3$**

Ferroelectricity in $BaTiO_3$ (Prevoskite)



Above 120 °C, $BaTiO_3$ has cubic structure. In a unit cell

Ba^{2+}---------Centre

Ti^{4+}---------Cube corner

O^{2-}----------Centre of cube edges

Fractional co-ordinates are

Ti(0,0,0)

Ba(1/2,1/2,1/2)

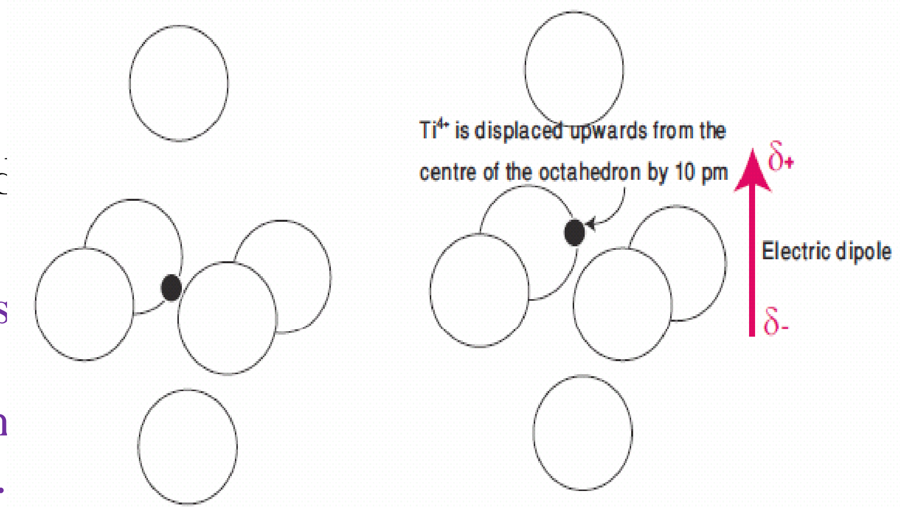
O(1/2,0,0), (0,1/2,0), (0,0,1/2)

Ti-ion (75pm)-----surrounded by octahedron of O_{2-}

Cubic Phase is non-ferro-electric

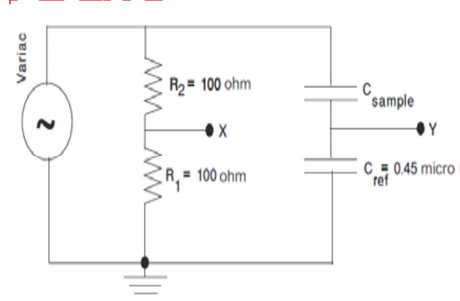
Tetragonal phase of $BaTiO_3$ (ferroelectric phase)

- At 120 °C------Cube----distort----TiO_6 group----distort
- Ti^{4+} ion displaces along a Ti-O bond axis.
- This displacement of Ti^{4+} ion causes non-overlap of the positive and negative charge centers, resulting in permanent electric dipole moment.

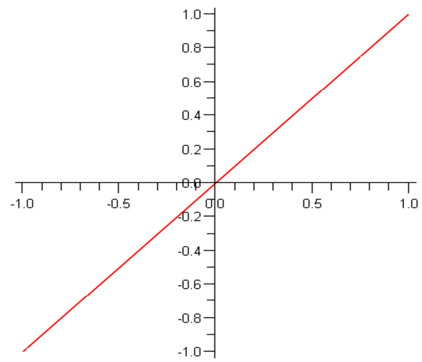


Neighboring domains have electric polarization that are either 90 or 180 degree w.r.t each other.

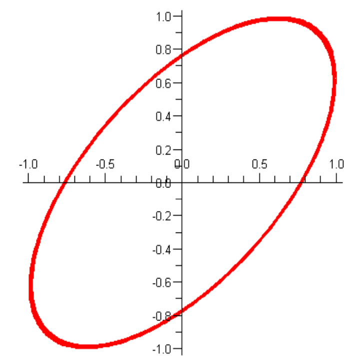
Maple simulation of RC-parallel circuit



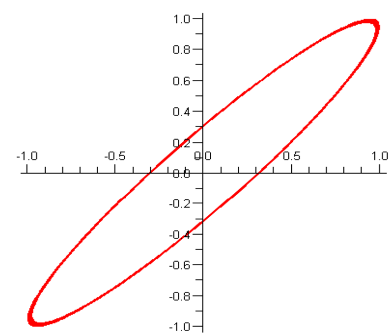
$$plot([cos(2 \cdot t),\ cos(2 \cdot t),\ t = -\pi..\pi])$$



$$plot\left(\left[cos(2 \cdot \pi \cdot 10 \cdot t),\ cos\left(2 \cdot \pi \cdot 10 \cdot t + \frac{\pi}{2} - \frac{1}{tan(1000)}\right),\ t = 0..10\right]\right)$$

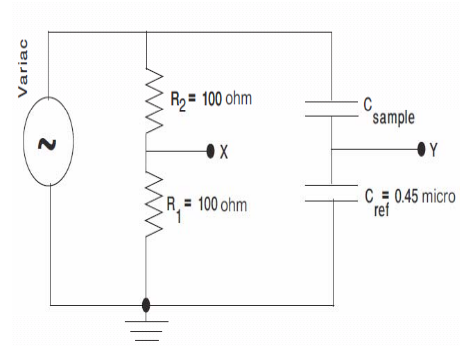


$$plot\left(\left[cos(2 \cdot \pi \cdot 10 \cdot t),\ cos\left(2 \cdot \pi \cdot 10 \cdot t + \frac{\pi}{2} - \frac{1}{tan(500)}\right),\ t = 0..10\right]\right)$$

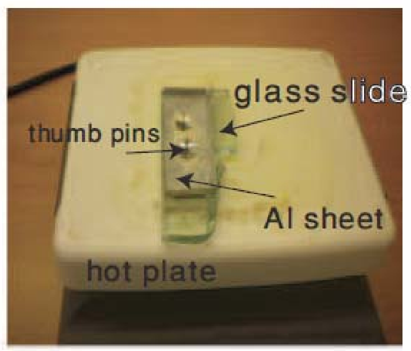


Development of Sawyer Tower Circuit

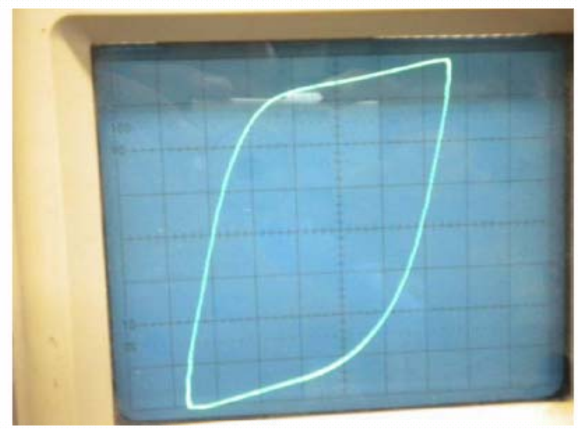
$BaTiO_3$ has a melting point of 1650°C while KNO_3 melts at 330°C. It is easy to make thin film of KNO_3 by melting as compared to $BaTiO_3$. Be warned that KNO_3 is a strong hydrophilic and water kills the ferroelectricity of the material, so before use the nitrate must be dried in a conventional microwave oven for about two minutes. KNO_3 is highly conductive in the molten state, so extreme care must be taken when it is dried in the microwave oven. Do not overheat, as arcing may occur in the molten conductive state of the salt.



(a)



(b)



Ferroelectric loop at 110˚C

Future Plan

- **Designing of Sawyer Tower Circuit for all kind of ferroelectric materials.**
- **Depositing ferroelectric thin films with spin-coater**
- **Studying ferroelectric loops at different frequencies.**

Thanks with

Good Energy!