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## **ENGINEERING PHYSICS**

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# ENGINEERING PHYSICS

## Unit 5 : Quantum mechanical treatment of Magnetic materials and Dielectrics



Class # 54

- *Polarization mechanisms in dielectrics*
- *Non Linear dielectrics - BaTiO<sub>3</sub>, structure and origin of non-centro symmetry of charges, phase changes*
- *Piezo electric materials - Pyro electric materials properties and applications*
- *Ferro electric hysteresis and application as memory materials*

### Class #54

- *Non linear dielectrics*
- *Crystal structures - point groups*
- *Classification of dielectrics*
- *BaTiO<sub>3</sub> structure*
- *Phase changes in BaTiO<sub>3</sub>*

# ENGINEERING PHYSICS

## Non linear dielectrics- BaTiO<sub>3</sub> structure and phase changes

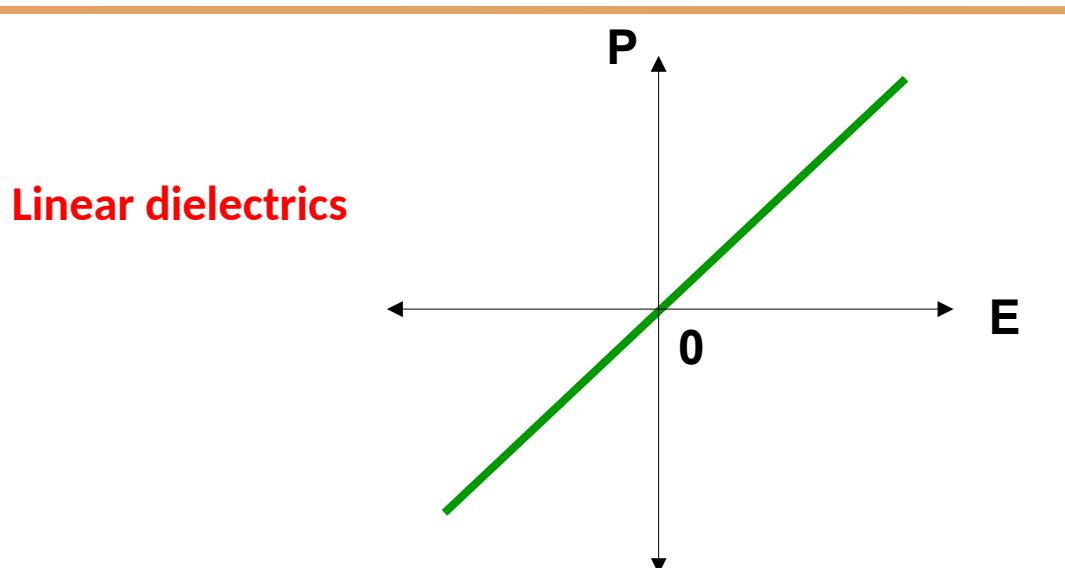


### ➤ Suggested Reading

1. *The Science and Engineering of Materials, Sixth Edition, Chapter 19, Donald R. Askeland, Pradeep P. Fulay and Wendelin J. Wright, 2010, Cengage Learning, Inc.*
2. *Learning material prepared by the Department of Physics*

## Non linear dielectrics

- *Polarization increases with the increase in applied field (E)*
- *In linear dielectrics, polarization (P) is linearly related to E and dielectric constant ( $\epsilon_r$ ) is constant*
- *Nonlinear dielectrics : E and P are not linearly related*



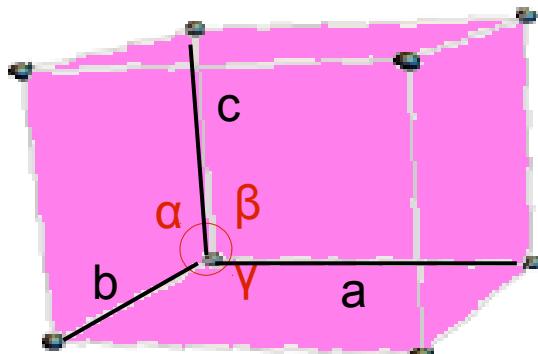
## Unit cell

- A crystal is a solid material having long range order with periodic structure
- Crystalline lattice: periodic pattern
- Unit cell : What is repeated
- Unit cell is characterized by lattice parameters

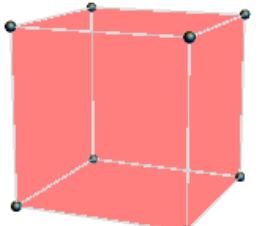


Corundum crystal

Source: Wikipedia

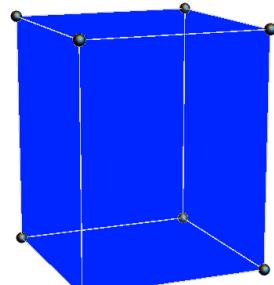
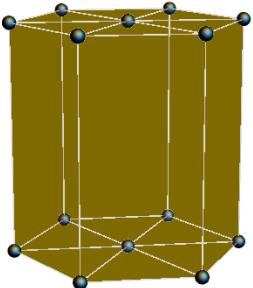


## Crystal systems



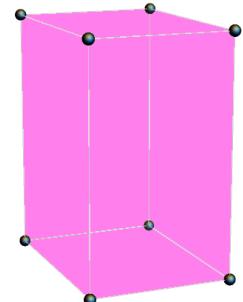
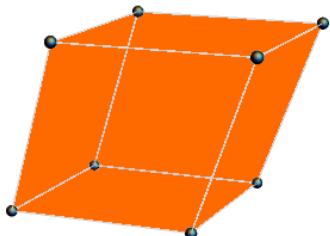
Cubic ;  $a=b=c$ ;  
 $\alpha=\beta=\gamma=90^\circ$

hexagonal ;  $a=b\neq c$ ;  
 $\alpha=\beta=90^\circ, \gamma=120^\circ$



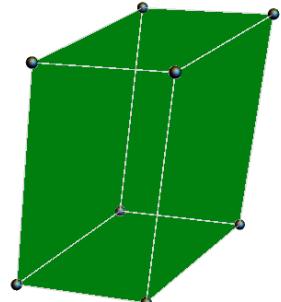
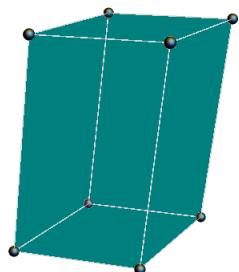
tetragonal;  $a=b\neq c$ ;  
 $\alpha=\beta=\gamma=90^\circ$

trigonal ;  $a=b=c$ ;  
 $\alpha=\beta=\gamma\neq 90^\circ$



Orthorhombic;  $a\neq b\neq c$ ;  
 $\alpha=\beta=\gamma=90^\circ$

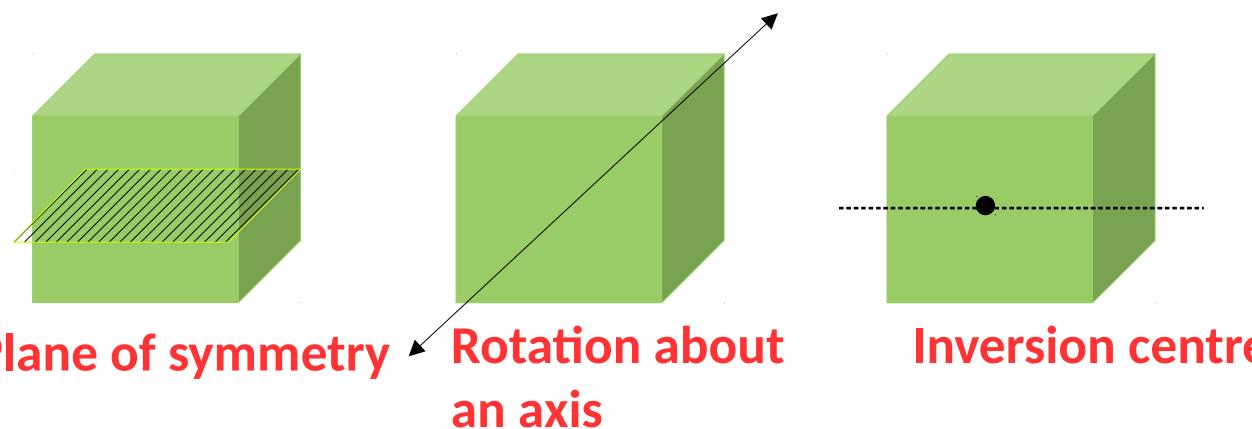
monoclinic;  $a\neq b\neq c$ ;  
 $\alpha=\beta=90^\circ\neq\gamma$



triclinic;  $a\neq b\neq c$ ;  
 $\alpha\neq\beta\neq\gamma$

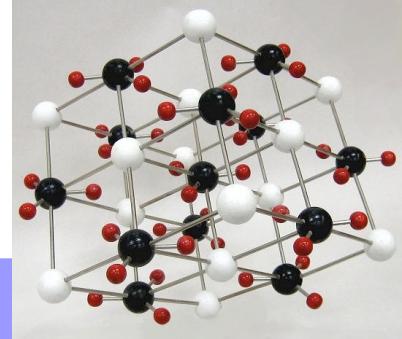
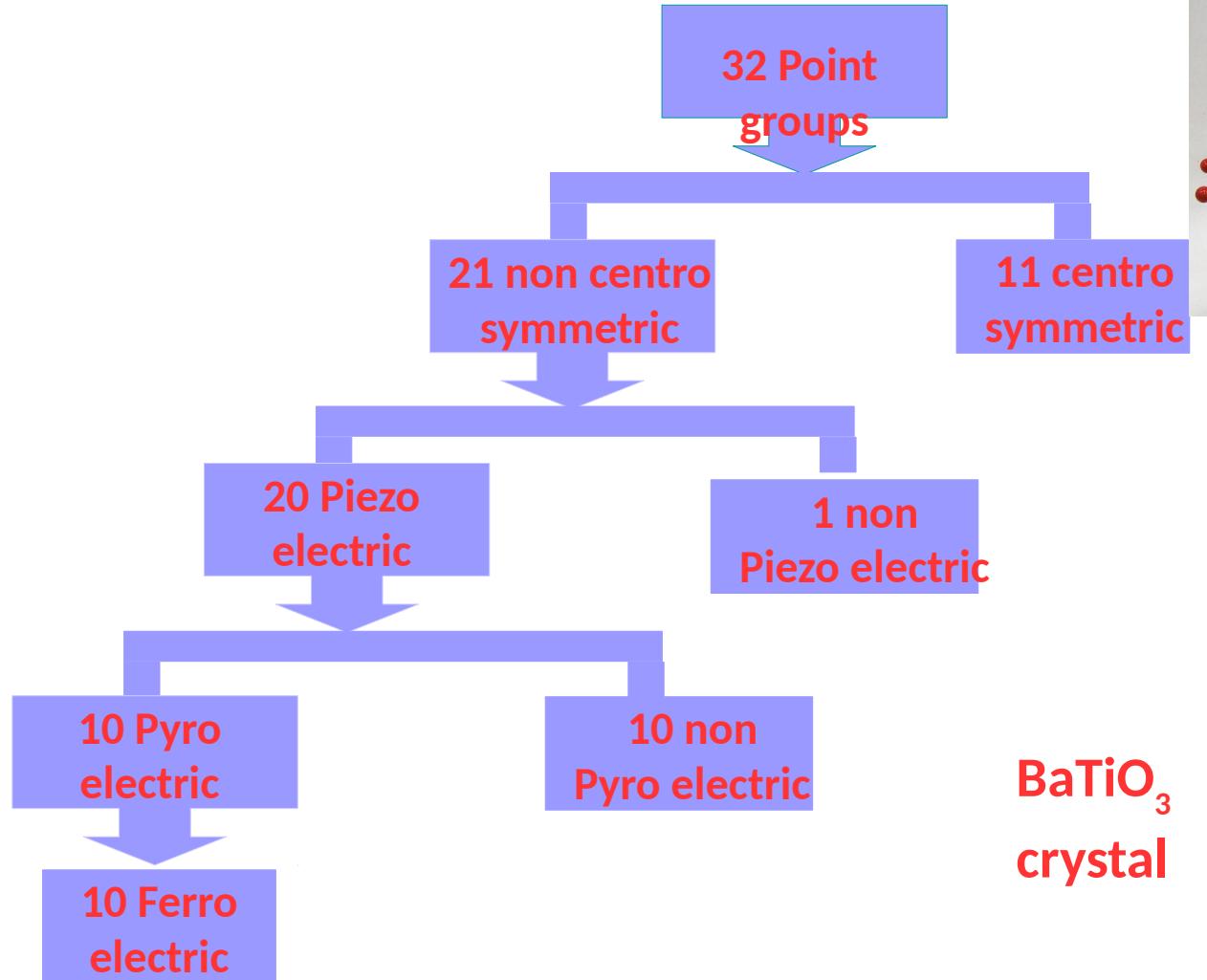
## Point groups

- *Orientation of crystal can be changed without seeming to change the positions of its atoms*
- *Changes of orientation: operations of reflection in a plane, rotation about an axis and inversion about a centre*
- *Point groups: 32 such distinct combinations*
- *Centro symmetric crystal: Centre of symmetry exists*



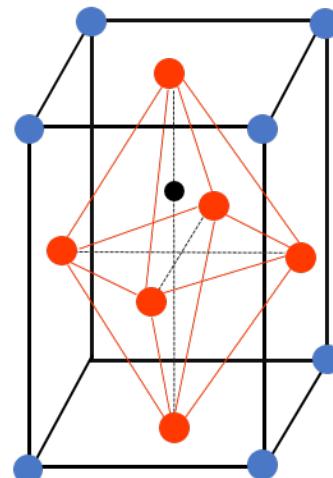
## Classification of dielectric materials

**Electrostriction: Polarization inducing a mechanical strain**



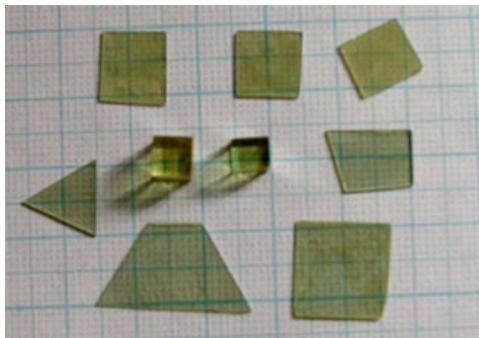
$\text{CaCO}_3$  crystal  
- Trigonal

$\text{BaTiO}_3$   
crystal



## Barium titanate – origin of non centro symmetry of charges

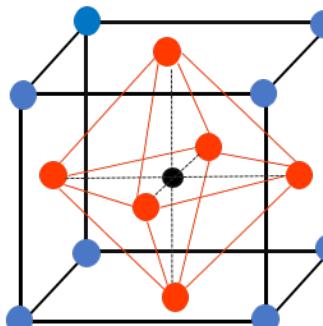
- *BaTiO<sub>3</sub> discovered in 1940's*
- *It has extremely high relative permittivity*
- *It is a non centro symmetric crystal - pervoskite*
- *Ba<sup>2+</sup> are located at the corners , Ti<sup>4+</sup> at the centre of the unit cell, octahedrally coordinated by six O<sup>2-</sup>*



Single crystal

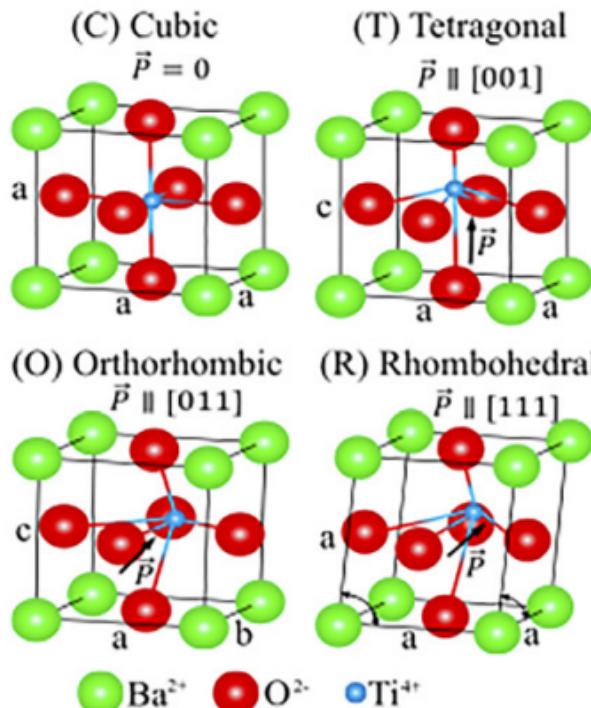
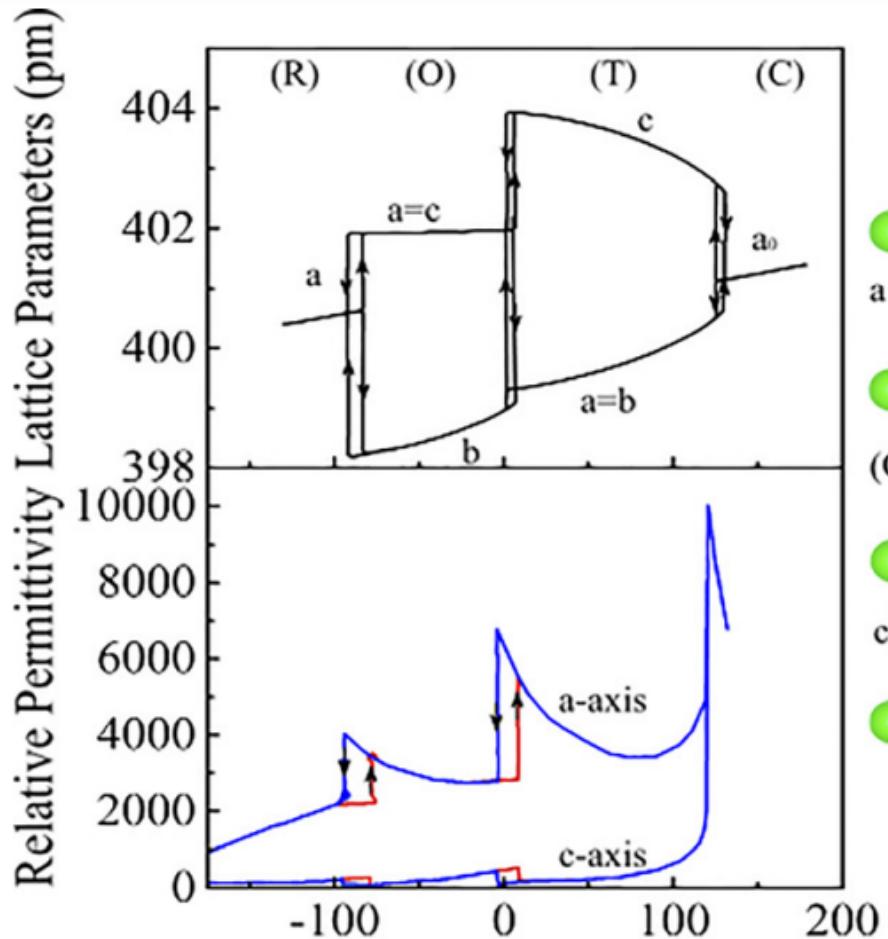
<http://www.crystal-material.com/Single-Crystal-Materials/Barium-titanate-BaTiO3-single-crystal.html>

● Ba<sup>2+</sup> ● O<sup>2-</sup> ● Ti<sup>4+</sup>



Unit cell in cubic phase

## Phase changes in $\text{BaTiO}_3$



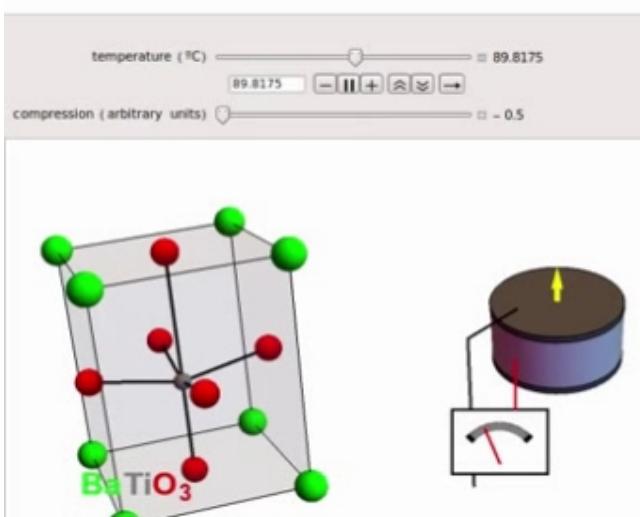
Curie temperature-  
**120°C**

Source:

<https://aip.scitation.org/doi/pdf/10.1063/1.4990046>

## Phase changes in BaTiO<sub>3</sub>

- All phases exhibit ferroelectric behaviour to some extent except cubic
- Cubic phase: paraelectric
- Tetragonal BaTiO<sub>3</sub>: Ferroelectric: An average relative displacement along the c-axis of titanium



**The concepts related to this class which are true are .....**

- 1. Dielectrics in which dielectric constant do not change with applied field are known as non linear dielectrics**
- 2. Unit cell is same for all the crystal structures**
- 3. Barium titanate at temperatures greater than 120°C is centro symmetric**
- 4. Displacement of titanium ions give rise to non centro symmetric behaviour in  $\text{BaTiO}_3$**
- 5.  $\text{BaTiO}_3$  can exist in cubic, orthogonal, monoclinic or tetragonal phases depending on its temperature**
- 6. All phases of  $\text{BaTiO}_3$  exhibit ferroelectric behaviour to some extent**



**THANK YOU**

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