Barium Titanate

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Abstract

Barium Titanate is a ferroelectric material. The study of Barium Titanate enables us to better understand ferroelectric phenomenon. Ceramics of Barium titanate can be polarized in a particular direction and used for various purposes. Various physical properties of single crystal of Barium Titanate are described in this article.

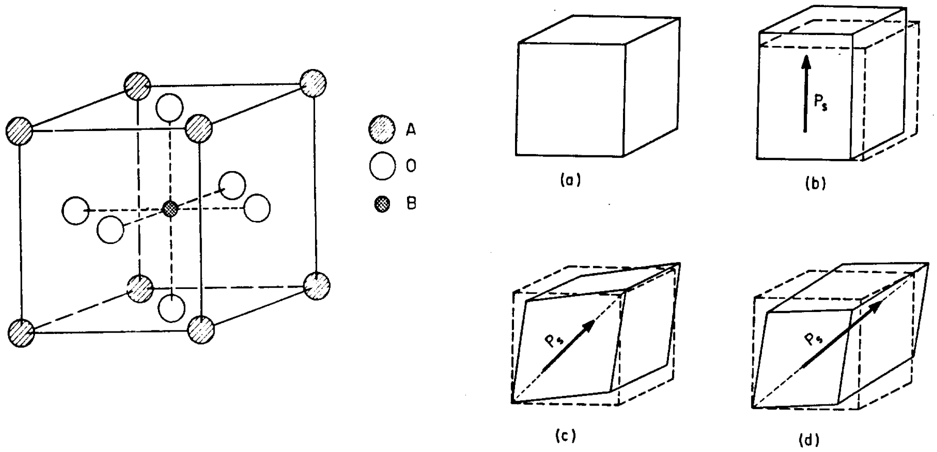

Figure 1: (i)Cubic Structure of Barium titanate($BaTiO_3$) with general formula ABO_3 (ii)Unit cells of four phases of Barium Titanate(a)cubic above 120^{o}C (b)Tetragonal (c) Orthorhombic (d) Rhombodedral[1]

1 Introduction:

Barium Titanate(BT) is a dielectric crystelline material which exhibits the anamalous properties typical for ferroelectricity. The ferroelectric activity of BT was reported in 1945-46 by Von Hippel and coworkers. BT is interesting from the view point of practical applications,firstly because it is chemicallly and mechanically very stable, secondly because it exhibits ferroelectric properties at and above room temperature and it can be easily prepared and used in the form of ceramic polycrystalline samples. The first single crystals of BT were produced in Switzerland in 1947.

2 Structure

The structure of BT belongs to the hexagonal system and perovskite-type.The perovskite-type crystal is stable below 1460^{o}C and becomes ferroelectric below 130^{o}C (Curie point). It belongs to the cubic system below 130^{o}C and its unit cell contains one molecular unit of BT Fig 1(i).

The symmetry of the polar phase,i.e; the phase below 130^{o}C, is tetragonal, with point group 4mm. In this state the crystal spontaneously acquires an electric polarization(a permanent electric dipole moment). As the polarization can in general point in any one of the originally cubic crystal axes, the crystal consists, in the ferroelectric state, of regions(domains) which differ in the direction of the spontaneous polarization. An applied electric field can align the polarization in the whole crystal and can reverse the polarization whereby electric hysteresis occurs. At lower temperatures, 5^{o}C and -90^oC, additional phase transitions take place.The spontaneous polatization successively changes its direction relative to the crystellographic axes and increases in absolute value. The direction of

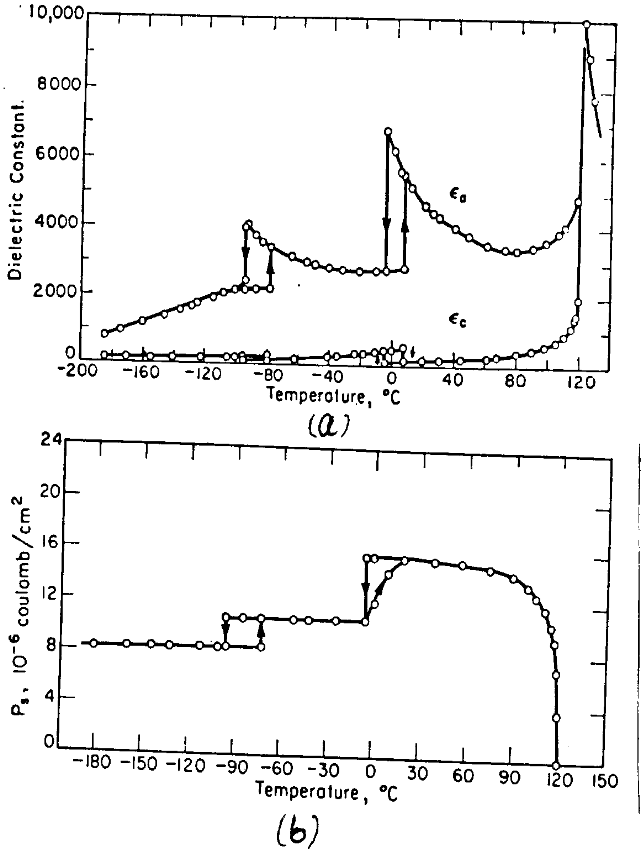

Figure 2: (a)Dielectric connstants of Barium Titanate as a function of temp.(b) Spontaneous polarization of BT,measured along the pseudo-cubic edge as a function of temp.[4]

polarization,from the high temperature end, are (100), (110) and (111) in terms of crystal system.the crystal belongs, in above order, to tetragonal, orthorhombic and rhombohedral systems[2]

3 Dielectric Properties:

In cubic phase there is only one principle dielectric constant, while in the tetragonal phase there are two[2]. BT has large dielectric constant in the vicinity of Curie point

$\epsilon = \epsilon_0 + C/(T - T_0)$

where ϵ_0 is the part of the dielectric constant independent of temperature, C Curie-Weiss constant, T temperature and To Curie point.

The field dependence of dielectric constant of BT can be found in [3]. The refractive index of the cubic phase is unusually large n = 2.4, it is temperature dependent. The refractive index of tetragonal phase is practically independent of temperature and shows no anomaly at the Curie point. In the cubic phase, the refractive index increases with decreasing temperature indicating that the electric polatizability increases as the Curie point is approached from above.

4 The Spontaneous Polarization:

The temperature dependence of spontaneous polarization P_s of BT single crystal is shown in Fig2(b)

The experimental points were obtained from measurements of the spontaneous polarization along pseudo-cubic (100) direction, the magnitude of this vector is obtained by multiplying the corresponding values of fig-2 with Sqrt[2]. Similarly in the rhombohedral phase, the experimental results reported in fig-2 must be multiplied with $Sqrt3$ in order to obtain the magnitude on P_s. The spontaneous polarization at Curie point is discontinuous.The value of spontaneous polarization at room temperature is $26 * 10^-6C/cm^2$.

5 The Coercive Field:

The hysteresis loops of good single crystals of BT exhibit rather sharp corners and a marked rectangular appearence. The value of corcive field, mearured at room temp, varies from a minimum of 500 V/cm to a maximum of about 2000 V/cm[M2]. These experimental values are much smaller than the value expected on the basis of the thermodynamic theory. The theoretical value is of the order of 10^5 V/cm. THe relatively small expt. values of the coercive field tell us that the crystal actually leaves a metastable state long before this state becomes unstable.

6 Specific heat and lattice distortion

The Curie trnaition in BT is of the first order therefore it should characterized by a latent heat. However , the specific heat measurements do not indicate abrupt changes. THis is due to the fact that internal strains, surface effects, temp inhomogeneities and other causes cooperate in spreading the anamalous heat changes over a finite temp range. The three phase changes occuring in BT are characterize by an expansion of the original cubic lattice in the direction of spontaneous polarization and a contraction in the direction perpendicular to it. BT is not piezoelectric in the non-polar phase compared to similar materials. When electric field is applied to the crystal, it produces strains proportional to the square of the field.

7 Lattice Vibration:

Information about the character of lattice vibrations and their change with temperature can be obtained from infrared and optical absorption studies. The most complete infrared absorption studiy is due to Last[5] who investigated BT and a no. of perovskite-type compounds. As there are five atoms in the cubic unit cell of BT, there are fifteen degrees of freedom, of which three are related to translational and three to torsional motion of the unit cell. The remaining nine modes aue associated with vibrational degrees of freedom.

The optical absorption edge of BT lies in the vecinity of 3800A and is only slightly affected by Curie transition at $120^{o}C$. This result might indicate that the electronic structure of BT does not undergo tadial changes at the Curie point.

Information about the effect of internal field on the degeneracy of the spin level can be obtained from the study of paramagnetic resonance in BT single crystals. Pure crystals, however, do not contain paramagnetic ions and therefore the effect was studied on BT crystals containing smallamount of paramagnetic impurities.

8 Uses:

Since BT has a high dielectric constant, typically 2000 for a ceramic sample at room temperature, capacitors of very small dimensions can be produced for electronic applications.

BT ceramics, when suitably doped with a trivalent oxide such as Lanthanul Oxide, for example, exhibit a variation of the electrical conductivity by a factor upto 10^6 in the vicinity of Curie-point .This effect can be used for sensitive temperature-control devices. Ceramics of BT and, in particular, of a mixed lead titanate zirconate can be poled by an electric field and retain a substantial remanent polarization. These materials then have a strong piezoelectric effect.In addition, they are mechanically rugged and rather insensitive to temperature and humidity. Therefore, these ceramics find wide applications in devices such as microphones, ultrasonic and underwater transducers, and spark generators.

References

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