# STRUCTURAL PHASE TRANSITION IN SOME PEROVSKITE MATERIALS HAVING POSITIVE THERMORESISTIVE COEFFICIENT (PTC)

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**Abstract**: Perovskite material $Ba_{0.946}Sr_{0.05}Y_{0.004}TiO_3$ having positive thermoresistive coefficient above room temperature was made by conventional ceramic method. The structure of the material was analyzed by X-ray diffractometer. The dependence of the dielectric constant, the total impedance on temperature and frequency was determined by a network analyzer. The anomalies of temperature dependence of the dielectric constant and the resistance are related to the structural phase transition. This phenomenon is explained basing on Landau phase transition theory.

## 1. Introduction

Ferroelectric perovskite materials basing on barium titanate ($BaTiO_3$) system have been widely studied contemporaneously for both basis and application interest (see [1]). It is well known that these materials undergo a second order phase transition from paraelectric (PE) to ferroelectric (FE) phase when temperature reduces from high value to lower than Curie temperature $T_C$. This PE-FE transition happens parallel with the structural phase transition from cubic to tetragonal crystal structure. Near $T_C$, some properties of doping ferroelectric crystals such as dielectric constant or resistivity show anomalies. In the present work, we study doped barium titanate perovskite $Ba_{0.946}Sr_{0.05}Y_{0.004}TiO_3$ which is a possible candidate for positive thermoresistive coefficient (PTC) thermoresistor. The anomalies of the dielectric constant and the resistivity of this material near phase transition are investigated.

## 2. Experiment

The ferroelectric perovskites can be produced by several ways such as hydrothermal reaction, sol-gel method... (See [1]). Here the basic polycrystalline $BaTiO_3$ and doped $Ba_{0.946}Sr_{0.05}Y_{0.004}TiO_3$ samples have been made by the conventional ceramic technology method. The prepared perovskite powders were pressed into pellets of 2 mm thick and 10 mm in diameter. The pellets were sintered at 1350 $^oC$ for 2 hours. Both the surfaces of samples were coated with Ag-Zn alloy by sputtering cathode method to form the electrodes. The structure of sintered bodies was analyzed by X-ray diffractometer D-5005 (Brucker). The temperature dependence of the sample resistance was measured using two-probe method. The Cole-Cole diagrams for real ($\varepsilon'$) and imaginary ($\varepsilon''$) parts of the complex dielectric constant of the sample were obtained by Network Analyzer MS 4630B in the frequency range from 30 kHz to 30 MHz. By using an equivalent circuit method for our material, the dependence of $\varepsilon'$ and $\varepsilon''$ on temperature and frequency was analyzed.

## 3. Results and discussion

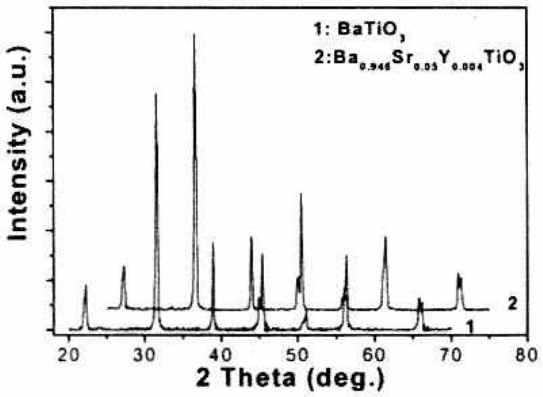


**Fig. 1.** X-ray diffraction pattern of samples

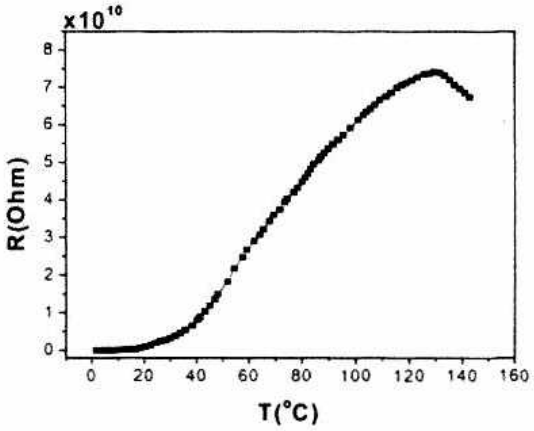


**Fig. 2.** Temperature dependence of resistance of doped sample

Fig. 1 shows the room temperature X-ray diffraction patterns for both sample types. We can see that the doping sample has the same structure as $BaTiO_3$. All peaks of the diffractogram were indexed on that of $BaTiO_3$. This indicates that doping sample is single-phase. At room temperature, the samples have a tetragonal structure with lattice constants given in table 1.

**Table 1:** Lattice parameters of doping sample and $BaTiO_3$

| Sample | a=b(Å) | c(Å) | c/a |
|---|---|---|---|
| $BaTiO_3$ | 3.992 | 4.030 | 1.0095 |
| $Ba_{0.946}Sr_{0.05}Y_{0.004}TiO_3$ | 3.970 | 3.990 | 1.010 |

The dependence of the sample resistance on temperature is showed in Fig. 2. It is seen from Fig. 2 that the doping sample presents very clearly the PTC effect and the region

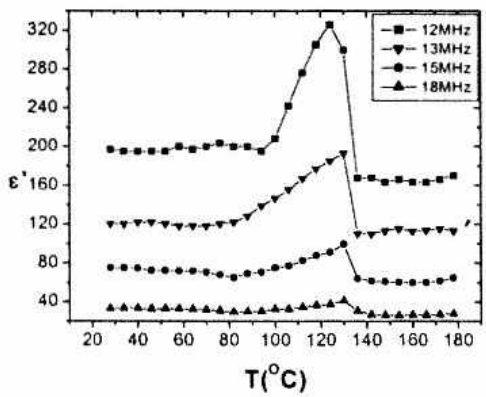


**Fig.3.** Temperature dependence of real part of dielectric constant of doped sample at various frequencies

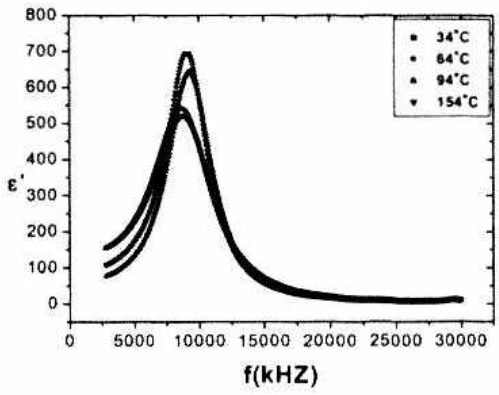


**Fig.4.** Frequency dependence of real part of dielectric constant of doped sample at various temperatures

for this effect spreads out from 40°C to 130°C. This linearity is very important for temperature sensor application. The maximum of resistance is rather high ~$7.10^{10}\Omega$ comparing with the composite perovskites [3]. The enormous change of resistance due to increasing temperature shows the smooth transition from semiconducting state to isolating one. Fig. 3 shows the temperature dependence of real part of dielectrical constant of $Ba_{0.946}Sr_{0.05}Y_{.0.004}TiO_3$ measured at various frequencies. This parameter has maximum at Curie temperature $T_C$~ 130°C and the maximum is more explicit for low frequency. This anomalous change of ε' is a specific feature of FE-PE transition. According to Landau, theory ([4], [1]) the static dielectrical constant ε has the anomaly temperature dependence $\varepsilon \sim |T - T_C|^{-1}$ near the second order phase transition point and this behavior is well illustrated in Fig. 3. Comparing Fig. 2 and Fig. 3, one sees that PTC effect mostly occurs in wide interval below $T_C$ (from 40°C to 130°C). Fig. 4 indicates that ε' has maximum around 10 MHz for measurement frequency interval from 0 to 30 MHz. Fig. 5 presents Cole-Cole diagrams of $Ba_{0.946}Sr_{0.05}Y_{0.004}TiO_3$ sample determined at several temperatures. These diagrams have a form of circle arcs showing that dielectrically media can be described by one relaxation time [1]. The reduction of ε' with increasing frequency from kHz to MHz ranges shows that the main contribution to the polarization in the studied material comes from ions. In conclusion, we can say that, doping $BaTiO_3$ by Sr and Y makes original isolating barium titanate become PTC material with potential for application.

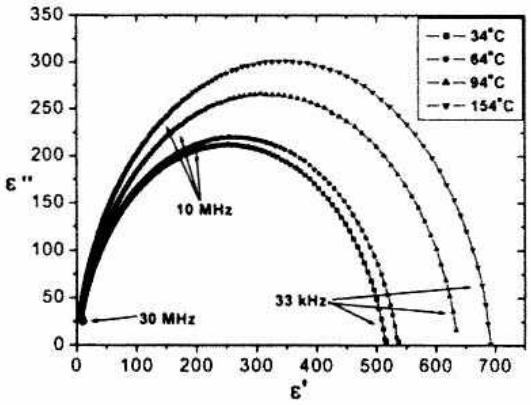


**Fig.5.** Cole-Cole diagrams of doped sample at various temperatures

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