

Effect of temperature on dielectric parameters of ferroelectric materials at microwave frequency

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Abstract

Background: The composite materials of ST and BT ceramics were prepared by using solid state reaction method. The dielectric parameters of ST and BT ceramics of particle size 125 micron like dielectric constant (ϵ'), loss (ϵ''), quality factor (QxF), relaxation time (τ) and conductivity (σ) has been studied at different temperatures i.e. -10°C , $+10^\circ\text{C}$, $+30^\circ\text{C}$ and $+50^\circ\text{C}$. the values of dielectric parameters are found greeter of ST then BT but the relaxation time of ST is found smaller than BT.

Keywords: dielectric constant (ϵ'), loss (ϵ''), quality factor (QxF), relaxation time (τ) and conductivity (σ), ST

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INTRODUCTION

SrTiO₃ belongs to the material class of the perovskites, ternary oxides of a structure ABO₃, where 'A' is mostly a group I, II element and 'B' is mostly a transition metal. The occupation of the 'A' and 'B' sites is very variable; Goodenough has reviewed more than 50 different perovskites. The cubic unit cell of SrTiO₃ with a lattice constant of 3.905. The octahedral corner-shared TiO₆ units form a tightly bonded network, which makes up the structural backbone of the lattice.¹⁻⁵ The chemical bonds in SrTiO₃ have a highly ionic character, but the covalent contribution to the titanium-oxygen bonds is not negligible. The perovskite structure is ideal for investigating the electronic structure of linear metal-oxygen-metal bonds of octahedrally coordinated metal ions. Direct metal-metal interactions are not possible due to an oxygen atom lying midway in between two titanium

neighbors. Oxygen-oxygen interactions are comparatively weak, since they have to get over distances twice as large as the titanium-oxygen bond lengths. In tight-binding descriptions of the perovskite electronic structure, interactions between atoms of the same element have often been considered weak enough to be treated as perturbations.⁶⁻⁸ In SrTiO₃, the influence of the highly ionized and electronically rather passive strontium ion on the titanium-oxygen covalence is small.⁹⁻¹¹ Relating the valence electronic structure to the atomic structure of a solid requires a physical description of the valence charge, which connects the atoms in the solid. The molecular orbital model is a description between as far as the strength of the interatomic interaction is concerned, the ligand field model, which applies to strictly localized electrons of weakly interacting atoms, and the band model, which applies to valence wave functions extended over many atoms.¹²⁻¹⁵ Considering a basic molecular orbital model for an isolated octahedral TiO₆ structural unit is instructive for interpreting the valence electronic structure of SrTiO₃. BaTiO₃ was discovered during World War II in 1941 and 1944 in the United States, Russia, and Japan. At least in the U.S.A., the research was accelerated because of the war. Most ferroelectric materials undergo a structural phase transition from a high-temperature nonferroelectric (or paraelectric) phase into a low-temperature ferroelectric phase. Some ferroelectrics, like barium titanate, BaTiO₃, undergo several phase transitions into successive ferroelectric phases.¹⁶ The

transition into a ferroelectric phase usually leads to strong anomalies in the dielectric, elastic, thermal. BaTiO₃ is a well-known ferroelectric and piezoelectric material having excellent dielectric properties. Its main application is as a dielectric in MLCC (Multi Layered Ceramic Capacitor) due to its high dielectric constant and low losses.¹⁷ The dielectric properties are controlled by purity

and microstructure which in turn is dependent on the method of preparation.¹⁸⁻²⁰

METHODOLOGY:

- Synthesis of material:** ST and BT ferroelectric materials were prepared by using SSR.

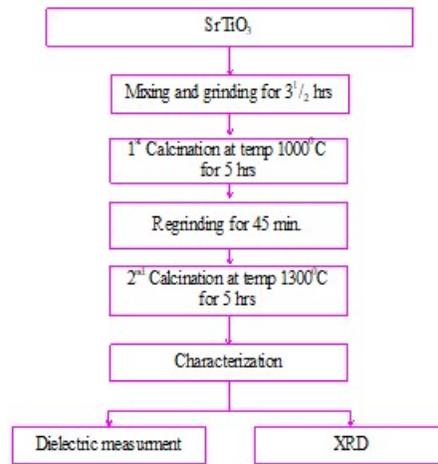


Figure 1: Flow Chart for Preparation of ST

RESULT AND DISCUSSION

The SrTiO₃ perovskite material synthesized by solid state reaction method is confirmed from the XRD which is matched with the JCPDF file no. (01-070-8508). ST material is obtained in the form of powder which is then separated in different particles size. The dielectric and physical parameter are determined by using x – band microwave bench having special designed solid cell. The reflectometric technique is used to determine accurate dielectric wavelength (λ_d). The Sharpness of BT diffraction peaks suggests better homogeneity and crystallization of the samples. The x-ray analysis indicates that the BaTiO₃ has single phase with tetragonal structure. All the reflection peaks were indexed using observed interplaner spacing d and lattice parameters with the JCPDS data of BT (Card no. 01-075-0460) were determined using a least squares refinement method. A good agreement between calculated and observed of values of all diffraction lines of BT suggests that (there is no change in the basic crystal structure) prepared sample is perovskite ferroelectric material and it useful for electro optic waveguide.

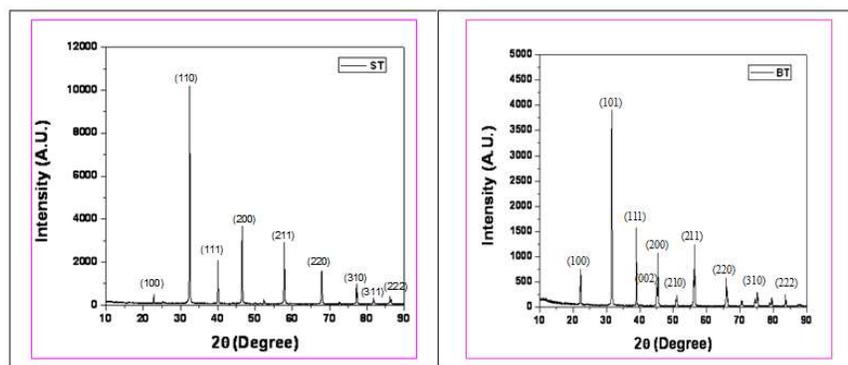


Figure 2: XRD pattern of SrTiO₃ and BaTiO₃

Table 1: Values of ε_p', ε_p'', Q, QxF, τ_p and σ_p of SrTiO₃ at different temperatures and particle sizes

Temp. (°c)	(δr)	ε' _p	ε'' _p	Q=1/tanδ	Q x F GHz	τ _p (P.S.)	σ _p
-10	0.90	18.52	2.85	0.153	6.53	64.32	2.47
	0.94	20.18	5.24	0.259	3.86	38.03	4.18
	0.98	23.70	7.16	0.302	3.31	32.61	4.88

10	1.00	29.26	9.08	0.310	3.22	31.77	5.01
	0.90	15.70	2.23	0.142	7.04	69.36	2.29
	0.94	17.54	3.86	0.220	4.54	44.77	3.55
	0.98	20.72	5.64	0.272	3.68	36.21	4.39
30	1.00	27.19	8.26	0.3004	3.28	32.40	4.91
	0.90	14.45	1.97	0.136	7.35	72.43	2.19
	0.94	15.82	2.84	0.180	5.55	54.72	2.91
	0.98	19.71	4.18	0.212	4.72	46.46	3.43
50	1.00	23.64	7.04	0.298	3.35	33.05	4.82
	0.90	13.00	1.72	0.132	7.58	74.62	2.13
	0.94	14.80	2.15	0.145	6.89	67.93	2.34
	0.98	18.12	3.16	0.174	5.74	56.60	2.81
	1.00	21.28	4.45	0.209	4.78	47.12	3.38

Table 2: Values of ϵ_p' , ϵ_p'' , Q, QxF, τ_p and σ_p of BaTiO₃ at different temperatures and particle sizes

Temp. (°C)	(δr)	ϵ_p'	ϵ_p''	Q=1/tan δ	Q x F GHz	τ_p (P.S.)	σ_p
-10	0.82	30.80	3.00	0.097	10.31	101.55	1.57
	0.88	42.12	5.02	0.119	8.40	82.74	1.92
	0.94	50.98	6.34	0.124	8.06	79.39	2.00
	1.00	62.72	8.28	0.132	7.57	74.56	2.13
10	0.82	23.46	2.14	0.091	10.98	108.15	1.47
	0.88	35.62	4.22	0.118	8.47	83.42	1.91
	0.94	42.14	5.18	0.122	8.196	80.73	1.97
	1.00	56.18	7.31	0.130	7.69	75.74	2.10
30	0.82	21.79	1.96	0.089	11.23	110.61	1.44
	0.88	31.00	3.36	0.108	9.25	91.11	1.74
	0.94	35.62	4.12	0.115	8.69	85.59	1.86
	1.00	51.26	6.14	0.119	8.40	82.74	1.92
50	0.82	19.44	1.66	0.085	11.76	115.83	1.37
	0.88	24.22	2.42	0.099	10.10	99.48	1.60
	0.94	29.76	3.26	0.109	9.17	90.32	1.76
	1.00	38.54	4.54	0.117	8.54	84.11	1.89

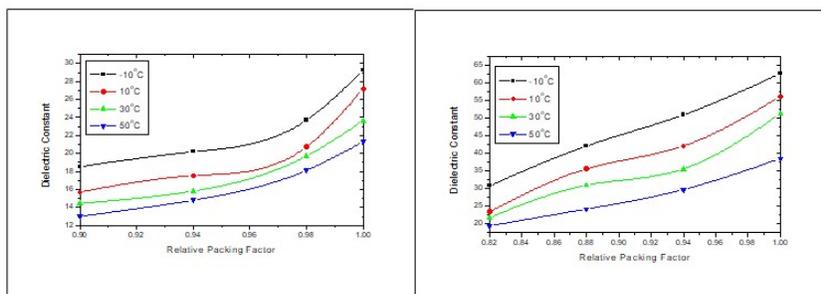


Figure 3: Dielectric Constant of ST & BT

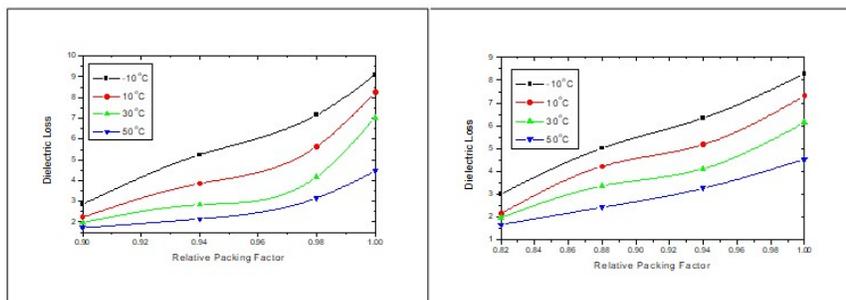


Figure 4: Dielectric Loss of ST & BT

CONCLUSION

In the present study of SrTiO₃ materials, the highest values of $\epsilon' = 29.26$ at $t = -10^\circ\text{C}$ and $\delta_r = 1$ and lowest value of $\epsilon' = 13$ at $t = 50^\circ\text{C}$ and $\delta_r = 0.90$. The dielectric constant value varies from 13 to 29.26. The value of ϵ' and ϵ'' are verified for solid bulk by using theoretical formulae of Bottcher's and Landu-Lifshitz-Looyenga. Then it is found at $\delta_r = 1$, the value of ϵ' and ϵ'' are nearly same. There is fair agreement between values obtained experimentally and theoretically. Hence it is proved that our assumption by taking lowest particle size powder of ST as solid bulk. From XRD of ST material, it is confirmed that the it is matched with JCPDF file no. 01-070-8508. From the crystal data of PDF card, the lattice parameters $a=3.903$, $b=3.903$, $c=3.903$ and crystal data axial ratio $c/a = 1$, $a/b = 1$, $c/b = 1$. The crystal symmetry of ST is found to be centro-symmetric. The sharp peak observed suggests the better homogenizing. The high intensity reflection peak is observed at an angle $2\theta=31.590$ (110) plane which is matched with angle $2\theta=32.4377$ (110) plane. Behavior of ϵ' and ϵ'' with δ_r and T: The graphical representation shows as the δ_r increases then ϵ' and ϵ'' are also increases systematically. It is due the density of BT material is to be increased material becomes more compact, as no voids are present. These values of ϵ' and ϵ'' are verified by using formulae of Bottcher's and L-L-L for solid bulk. The lowest particle size of 50 micron is considered as a solid bulk. It is found at $\delta_r = 1$, i.e. least particle size the values of ϵ' and ϵ'' are nearly same. Behavior of τ_r and σ_p with δ_r and temperature: As δ_r i.e. packing density of BT material increases the values of τ_r and σ_p are also increases. The values are maximum at least particle size. The values of τ_r and σ_p decreases by increasing the temperature. From X-Ray diffraction study of BT: All the highest intensity peaks of BT sample are listed out and compared with the standard JCPDF (No. 01-075-0460). It is found the values of Bragg's angle (2θ), Interplanar spacing (d), intensity (I) and miller indices (hkl) are nearly matched with the values of BT sample. In the present study of BaTiO₃ materials, the highest value of $\epsilon' = 62.72$ is observed at temperature = -10°C and at $\delta_r = 1$. The lowest value of $\epsilon' = 19.44$, found dielectric constant varies from 19.44 to 62.72 at temperature range (50°C , 30°C , 10°C , -10°C). There is fair agreement between the values obtained

experimentally and theoretically. Hence, the formulae of Bottcher's and L-L-L work well between powder and solid bulk. The crystal structure of BT material is orthorhombic. From PDF card, the crystal data as a lattice parameter are $a=3.994$, $b=3.994$, $c=4.034$ and crystal data axial ratio are $c/a=1.010$, $a/b=1.00$, $c/b=1.010$. The crystal symmetry of BT is centrosymmetric.

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