CHAPTER 3

GROWTH AND CHARACTERIZATION OF BARIUM STRONTIUM TITANATE SINGLE CRYSTALS

3.1 INTRODUCTION

$\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ (BST) is a ferroelectric-antiferroelectric solid solution and is one of the important ferroelectric as well as photorefractive materials. This material is used in electronic, electro-optical, acoustic and microwave devices (Outzourhit et al 1995). Potential applications include pyroelectric detectors, transducers, resonators, memory devices, capacitors, photorefractive mirrors (Zhuang et al 1991; Buse et al 1993), thermistors, sensors (Uusimaki et al 1982), under cooled detectors fabrication (Pandey 1994), positive temperature coefficient resistors (Ali and Milne 1993) and gate insulator for the oxide superconductor field effect transistor (Kobayashi and Kobayashi 1994). Most of the applications exploit the properties of the ferroelectric phase. The Curie point can be controlled accurately by changing the Sr concentration in BST. This change is accompanied by the dielectric properties that can be tailored for a specific applications at a given operating temperature. The photorefractive properties of BST can be used for many applications which include optical signal amplification, image processing, optical data storage, holography and self pumped phase conjugation. Several reports are available on the growth of BST single crystals. But only a few papers reported the ferroelectric characterization of BST single crystals. The present chapter deals with the growth of BST single crystals by high temperature solution growth technique. The variations in Curie temperature,
dielectric properties, lattice parameters and spontaneous polarization for different concentrations of Sr are also discussed.

3.2 PHASE DIAGRAM

The structure of this system is perovskite as discussed in chapter 2. The phase diagram of \( \text{BaTiO}_3 - \text{SrTiO}_3 \) constructed by Basmajian and De Vries (1957) and Wechsler and Kirby (1992) is shown in Figures 3.1 and 3.2 respectively. The above reports present controversial results. According to Basmajian and De Vries (1957), the system is a complete solid solution in which the composition of Sr can be obtained from 0 to 100 mol.%. It was also reported that \( \text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3 \) melts congruently at 2.5 mol. % of Sr. Wechsler and Kirby (1992) reported that the doping of \( \text{SrTiO}_3 \) results in a binary melting loop with liquidus and solidus temperatures rising in the direction of \( \text{SrTiO}_3 \). However the binary loop is interrupted because of the limited solubility of \( \text{SrTiO}_3 \) in hexagonal phase \( (\text{Ba},\text{Sr})\text{TiO}_3(\text{ss}) \). The maximum solubility of \( \text{SrTiO}_3 \) in hexagonal phase lies between 20 and 30 mol.% at 1631°C, where the invariant reaction hexagonal \( (\text{Ba},\text{Sr})\text{TiO}_3(\text{ss}) \leftrightarrow \text{cubic} \ (\text{Ba},\text{Sr})\text{TiO}_3 \ (\text{ss}) + \text{liquid} \) takes place. These results differ from the result of Basmajian and De Vries (1957), that there exist a melting point depression with Sr doping and a congruent melting point at about 2.5 mol.% of Sr. Later Buse et al (1993) reported that 1.6 atomic % of Sr is sufficient for the system to melt congruently. On increasing Sr concentration, the tetragonality decreases and the structure becomes cubic. There are controversial reports on the shifting of cubic phase with Sr content. Drust et al (1950) and McQuarrie (1955) reported the coexistence of cubic phase for a Sr concentration of 30 mol.% and above, whereas Barb et al (1982) showed that the cubic phase exists for 28 mol. % of Sr.
Figure 3.1 Phase diagram of BaTiO$_3$ - SrTiO$_3$ for complete solid solution.
Figure 3.2 Phase diagram of BaTiO$_3$ - SrTiO$_3$ for partial solid solution.
3.3 CRYSTAL GROWTH

Crystal growth of barium strontium titanate (BST) has been investigated by many workers. Growth of BST single crystals by flux growth (Balakumar et al. 1995; Khodakov et al. 1955; Coufova et al. 1972; Goulpeau 1975), Czochralski (CZ) growth (Nassau and Broyer 1962; Bethe and Welz 1971; Godfroy et al. 1980; Zhuang et al. 1991; Buse et al. 1993) and float zone technique (Brown and Todt 1964; Tien and Garretson 1972; Furukaa and Tsukamoto 1991; Kojima et al. 1995) has been reported. Because of the high melting point, it is very difficult to grow crystals with higher Sr concentration by Czochralski and float zone techniques. Hence the flux method is the only successful method for the growth of BST single crystals.

Single crystals of BST were grown from the precursor of BaCO₃ (Aldrich 99.99%), SrCO₃ (Aldrich 99.995%) and TiO₂ (Aldrich 99.9%) by Remeika’s method (Remeika 1954). The starting materials corresponding to composition Ba₁₋ₓSrₓTiO₃ (x = 5, 10, 15, 20 and 30 mol.%) were accurately weighed and thoroughly ground in an agate mortar using acetone. Then the charge was mixed with KF flux, and tightly closed in a 100 cc platinum crucible to avoid the flux evaporation. The growth runs were performed in a silicon carbide vertical type resistive heating furnace with precise temperature controller as discussed in chapter 2. Axial temperature gradient of 2-3°C/cm and a vertical gradient of 3-4°C/cm was maintained at the vicinity of the crucible. The furnace was heated to high temperature (1180 to 1250°C), homogenized for a few hours (10 to 36 hours), slow cooled to 800°C at a rate of 1-4°C/hr and finally cooled to room temperature at a rate of 75°C/hr. Most of the crystals were found at the bottom of the crucible. The crystals were separated from the flux by dissolving in hot water. Size and quality of the crystals are the main factors taken into account for the optimization of growth parameters. The growth parameters were optimized by changing the flux-charge ratio, cooling rate and soaking period and the optimized conditions are given in table 3.1.
The growth parameters, size and morphology of the crystals depend on the Sr concentration. For a Sr concentration of 5 mol. % and lower soaking period, platy crystals were obtained. The soaking period was increased and the cooling rate was decreased in order to grow good quality bulk crystals. On increasing the Sr concentration, the amount of flux was increased because of high melting point of SrTiO$_3$. The flux-charge ratio was changed and the optimum ratio was determined by trial and error method and the values are given in table 3.1. Crystals of size 5 x 5 x 3 mm$^3$ were obtained and the as-grown crystals for Sr concentration of 10, 15 and 20 mol. % are shown in Figures 3.3a, b and c respectively. On further increasing the Sr concentration (30 mol.% of Sr), the size of the crystals was reduced.

**Table 3.1**

<table>
<thead>
<tr>
<th>Starting composition</th>
<th>Flux-charge ratio</th>
<th>Growth temperature (°C)</th>
<th>Soaking period (hrs)/cooling rate (°C/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba$<em>{0.95}$Sr$</em>{0.05}$TiO$_3$</td>
<td>70:30</td>
<td>1180</td>
<td>7/5-8</td>
</tr>
<tr>
<td>Ba$<em>{0.85}$Sr$</em>{0.15}$TiO$_3$</td>
<td>75:25</td>
<td>1180</td>
<td>15/5-8</td>
</tr>
<tr>
<td>Ba$<em>{0.80}$Sr$</em>{0.20}$TiO$_3$</td>
<td>75:25</td>
<td>1200</td>
<td>20/3-5</td>
</tr>
<tr>
<td>Ba$<em>{0.70}$Sr$</em>{0.30}$TiO$_3$</td>
<td>85:15</td>
<td>1250</td>
<td>24/1-3</td>
</tr>
</tbody>
</table>

3.4 **SURFACE MORPHOLOGY**

Two types of surface features like vein and layer growth structures were observed on the as-grown crystals through an optical microscope. Supersaturation and cooling rate are the major factors which decide the growth mechanism. The vein structure is of two types as shown in Figures 3.4 a and b. Unlike in BCT, in the case of BST the veins are shorter in length and do not spread over the entire crystal surface (Figure 3.4a). This type of structure was observed on the crystals with 5 mol.% of Sr. Figure 3.4 b displays a different type of vein structure with thick veins. The veins
Figure 3.3  BST single crystals for Sr concentration 
(a) 10, (b) 15 and (c) 20 mol.%
Figure 3.4  Surface morphology of $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ (a) & (b) vein structure, (c) layer growth pattern
are filled by layers in between. This type of structure may be formed due to the lower supersaturation and the existence of hexagonal phase. Figure 3.4 c shows the layer growth structure observed on the crystal with higher concentration of Sr (20 mol.%). This type of layer growth mechanism occurs due to two dimensional nucleation and also due to higher supersaturation.

3.5 X-RAY DIFFRACTION STUDIES

3.5.1 Single crystal X-ray diffraction

Single crystal X-ray diffraction has been carried out to study the change in structure on Sr substitution. The X-ray data were collected at room temperature using a Philips PW1100 single crystal X-ray diffractometer with MoK\(_\alpha\) radiation (\(\lambda = 0.71069\) Å). For the data collection one standard reflection was monitored for every 100 times without significant variations. The diffraction data were corrected for Lorentz and for polarization effects during the data reduction procedure (Belletti 1996). After the isotropic refinement the data were corrected for absorption following the method of Walker and Stuart (1983) with a software written by Gluzinski (1989). The geometry of the molecules was determined by the Crysruler package (Rizzoli et al 1987) and the structure using Cerius 2 program (CERIUS\(^2\) 1997). The projected structure of the crystal is shown in Figure 3.5. The crystal characteristics and filling coefficients, thermal parameters are listed in table 3.2 and 3.3 respectively (Varatharajan et al 1999b).

3.5.2 Laue and powder X-ray diffraction

Figure 3.6 shows the reflection Laue photograph of BST single crystal grown with 20 mol.% of Sr. The spots are well defined and confirm the single crystallinity and also the good quality of the crystal. Figures 3.7a, b, c and d show powder X-ray diffraction pattern of the BST crystals with 10, 15, 20 and 30 mol.% of Sr respectively. It is confirmed that crystals possess perovskite structure. The lattice parameters were calculated and found to decrease on increasing the Sr concentration.
Figure 3.5  Structure of BST single crystal
Figure 3.6  X-ray Laue back reflection photograph of Ba$_{0.8}$Sr$_{0.5}$TiO$_3$ crystal
Figure 3.7 Powder X-ray diffraction pattern of (a) Ba$_{0.5}$Sr$_{0.15}$TiO$_3$, (b) Ba$_{0.85}$Sr$_{0.15}$TiO$_3$
Figure 3.7  Powder X-ray diffraction pattern of (c) Ba$_{0.80}$Sr$_{0.20}$TiO$_3$, (d) Ba$_{0.70}$Sr$_{0.30}$TiO$_3$
This is due to the lower ionic radius of Sr compared to Ba. The c/a ratio declines on Sr doping and hence the tetragonality of the system. For 30 mol.% of Sr the system shifts to paraelectric cubic phase. The lattice parameter values are tabulated in 3.4.

<table>
<thead>
<tr>
<th>Table 3.2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Single crystal X-ray diffraction data of Ba$_{1-x}$Sr$_x$TiO$_3$ (x = 0.2, 0.3)</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Monogram</th>
<th>Ba$<em>{0.8}$Sr$</em>{0.2}$TiO$_3$</th>
<th>Ba$<em>{0.7}$Sr$</em>{0.3}$TiO$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal dimensions (mm$^3$)</td>
<td>0.1 x 0.2 x 0.2</td>
<td>0.2 x 0.3 x 0.4</td>
</tr>
<tr>
<td>n°of reflections θ Range (°)</td>
<td>31 5.1-39.9</td>
<td>46 7.3-40.1</td>
</tr>
<tr>
<td>Cell volume (Å$^3$)</td>
<td>63.95</td>
<td>63.14</td>
</tr>
<tr>
<td>Collected reflections</td>
<td>265</td>
<td>259</td>
</tr>
<tr>
<td>Unique reflections Rint</td>
<td>63 0.09</td>
<td>62 0.12</td>
</tr>
<tr>
<td>Obs.Refl.[I&gt;2σ(I)]</td>
<td>63</td>
<td>62</td>
</tr>
<tr>
<td>θ range (°)</td>
<td>3-40</td>
<td>3-40</td>
</tr>
<tr>
<td>Indices range : h,k,l</td>
<td>0-4, 0-5, 1-7</td>
<td>0-4, 0-5, 1-7</td>
</tr>
<tr>
<td>No.of refined parameters</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>R (for obs. refl.)</td>
<td>0.0228</td>
<td>0.0125</td>
</tr>
<tr>
<td>R (for all refl.)</td>
<td>0.0228</td>
<td>0.0125</td>
</tr>
<tr>
<td>R$_w$</td>
<td>0.055</td>
<td>0.0197</td>
</tr>
<tr>
<td>W=1[(σ$^2$Fo$^2$+(KP)$^2$) +YP] K,Y</td>
<td>0.0, 0.50</td>
<td>0.002, 0.0</td>
</tr>
<tr>
<td>GOF</td>
<td>1.19</td>
<td>0.86</td>
</tr>
<tr>
<td>$\rho_{min/max}$</td>
<td>-2.30/1.91</td>
<td>-4.10/1.81</td>
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Table 3.3

Filling coefficients (%) of atoms in the different sites of the molecules.

<table>
<thead>
<tr>
<th>Site</th>
<th>Element</th>
<th>(\text{Ba}<em>0.8\text{Sr}</em>{0.2}\text{TiO}_3)</th>
<th>(\text{Ba}<em>0.7\text{Sr}</em>{0.3}\text{TiO}_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>Ba</td>
<td>82.4</td>
<td>99.8</td>
</tr>
<tr>
<td></td>
<td>Sr</td>
<td>17.6</td>
<td>17.6</td>
</tr>
<tr>
<td>1b</td>
<td>Ti</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>3c</td>
<td>O</td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>

Anisotropic and isotropic thermal parameters (x10^4 Å²) for \(\text{Ba}_0.8\text{Sr}_{0.2}\text{TiO}_3\)

\(U_{ij}\) are in the form \(\exp(-2.\pi.U_{11}.h^2.a^*+...+2.U_{12}.h.k.a^*^2.b^*^2+...)\)

<table>
<thead>
<tr>
<th></th>
<th>(U_{11})</th>
<th>(U_{22})</th>
<th>(U_{33})</th>
<th>(U_{23})</th>
<th>(U_{13})</th>
<th>(U_{12})</th>
</tr>
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<tbody>
<tr>
<td>Ba/Sr</td>
<td>10 (3)</td>
<td>10 (3)</td>
<td>10 (3)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ti</td>
<td>36 (7)</td>
<td>36 (7)</td>
<td>36 (7)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>O1</td>
<td>38 (20)</td>
<td>34 (13)</td>
<td>34 (13)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Anisotropic and isotropic thermal parameters (x10^4 Å²) for \(\text{Ba}_0.7\text{Sr}_{0.3}\text{TiO}_3\)

\(U_{ij}\) are in the form \(\exp(-2.\pi.U_{11}.h^2.a^*+...+2.U_{12}.h.k.a^*^2.b^*^2+...)\)

<table>
<thead>
<tr>
<th></th>
<th>(U_{11})</th>
<th>(U_{22})</th>
<th>(U_{33})</th>
<th>(U_{23})</th>
<th>(U_{13})</th>
<th>(U_{12})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba/Sr</td>
<td>11 (17)</td>
<td>11 (17)</td>
<td>11 (17)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ti</td>
<td>10 (32)</td>
<td>10 (32)</td>
<td>10 (32)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>O1</td>
<td>71 (132)</td>
<td>67 (84)</td>
<td>67 (84)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

3.6 FERROELECTRIC STUDIES

3.6.1 Domain structure studies

The spontaneous polarization \(P_s\) can lie along any of the three directions which are equivalent in the cubic phase. Thus the tetragonal phase has adjacent regions which are polarized at 90° to each other, called 90° domains as shown in Figure 3.8a. The condition for the formation of such domains is the continuity and the...
matching of lattice at the boundary. Such condition is fulfilled by the geometry shown in Figure 3.8b. It is apparent from the Figure 3.8b that the angle between the polar c-axis of the adjacent domains has a slight variation from 90° which can be estimated from the geometric condition $2\tan^{-1}(c/a)$, where $a$ and $c$ are lattice parameters. Taking $c/a = 1.01$ for BaTiO$_3$, the deviation angle is found to be about 0.6° (Takashige et al 1996).

The domain structure of BST single crystals was observed using Atomic Force Microscope (Nanoscope II). The experimental conditions are the same as discussed in chapter 2. Figure 3.9 shows the AFM image of 90° c- domains. The deviation angle was calculated from the cross section profile and is found to be in the range 0.3 to 0.45°. For BST single crystal with 10 mol.% of Sr, the angles are comparable with the lattice parameters.

### 3.6.2 Hysteresis studies

Hysteresis, the real identity of a ferroelectric material, has been studied for the crystals with Sr concentration of 10, 15, 20 and 30 mol.% as shown in Figures 3.10a, b, c and d respectively using a Sawer-Tower circuit. The hysteresis loops obtained are well defined having perfect structure. This confirms the good quality of the grown crystals. For Ba$_{0.7}$Sr$_{0.3}$TiO$_3$, as shown in Figure 3.10d, the structure of the loop is not a perfect square indicating that the system shifts to paraelectric cubic phase. The spontaneous polarization $P_s$ values were calculated from hysteresis. The $P_s$ values rapidly decrease on increasing Sr concentration and this may be due to the antiferroelectric nature of SrTiO$_3$. The spontaneous polarization values for different concentrations of Sr are presented in table 3.4.
Figure 3.8a  Schematic of 90° domain structure of tetragonal BaTiO₃

Figure 3.8b  Schematic conditions for matching of the lattice at the 90° domain boundary
Figure 3.9  AFM image of 90° domains
Figure 3.10  Hysteresis loops of (a) $\text{Ba}_{0.90}\text{Sr}_{0.10}\text{TiO}_3$, (b) $\text{Ba}_{0.85}\text{Sr}_{0.15}\text{TiO}_3$
(c) $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$ and (d) $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$
3.6.3 Dielectric studies

Dielectric properties of ceramic and single crystals of BST have been extensively studied by Jaffe et al (1971); Barb et al (1982); Syamaprasad et al (1988); Kazaoui and Ravez (1991); Yasuda et al (1994). It has been reported that the ferroelectric to paraelectric transition is sensitive to Sr concentration. The transition temperature decreases linearly with increasing Sr concentration (Jaffe et al 1971). The ferroelectric phase transition was reported to be diffused for both ceramics as well as single crystals (Bethe and Welz 1971; Benguigui and Bethe 1978; Syamaprasad et al 1988). Figures 3.11, 3.12, 3.13 and 3.14 show the temperature Vs dielectric constant for the BST crystals grown with 10, 15, 20 and 30 mol.% of Sr. It has been observed that the dielectric constant reaches a maximum at the Curie temperature and then starts decreasing. It has also been observed that the dielectric constant decreased on increasing Sr concentration in agreement with Yasuda et al (1994). The e value reaches a maximum of 1000 for 30 mol.% of Sr which is 10 times less than that of BaTiO3. This result is in good agreement with Khodakov et al (1955) and Coufova et al (1972). This reduction in dielectric constant is due to the doping of antiferroelectric SrTiO3 in ferroelectric BaTiO3 (Verbitskaya et al 1988). In the present investigation, as grown BST single crystals showed pronounced change in the ferroelectric properties.

The Curie temperature decreases on increasing the Sr concentration as shown in table 3.4. Like barium calcium titanate, BST single crystals also showed diffused phase transition (DPT) behaviour as shown in Figures 3.11, 3.12, 3.13 and 3.14. The diffused nature increased while increasing the Sr concentration as reported by Benguigui and Bethe (1978). The diffused phase transition behaviour is similar to the observations on Ba1.xCa0.2TiO3 (Varatharajan et al 1998), PbMg1/3Nb2/3O3 (Kirilov and Isupov 1973), Pb(Sc0.5Tao.5)O3 (Stenger et al 1979) and (Pb,La)(Zr,Ti)O3 (Stenger and Burggraaf 1980). The occurrence of DPT may be due to the intrinsic disorder
Figure 3.11  Dielectric constant Vs Temperature for $\text{Ba}_{0.9}\text{Sr}_{0.1}\text{TiO}_3$
Figure 3.12  Dielectric constant Vs Temperature for Ba$_{0.85}$Sr$_{0.15}$TiO$_3$
Figure 3.13  Dielectric constant Vs Temperature for $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$
Figure 3.14  Dielectric constant Vs Temperature for Ba$_{0.7}$Sr$_{0.3}$TiO$_3$
effect introduced by the replacement of Ba$^{2+}$ by Sr$^{2+}$ similar to BCT single crystals and other solid solutions (Tiwari et al 1989; Cross 1987).

Table 3.4

The lattice parameter values, $P_s$ and $T_c$ for $Ba_{1-x}Sr_xTiO_3$ single crystals

<table>
<thead>
<tr>
<th>Starting composition</th>
<th>Lattice parameters</th>
<th>$P_s$ ($\mu$m/$cm^2$)</th>
<th>$T_c$ ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$a$ (Å)</td>
<td>$c$ (Å)</td>
<td></td>
</tr>
<tr>
<td>$Ba_{0.95}Sr_{0.05}TiO_3$</td>
<td>3.997</td>
<td>4.011</td>
<td>21.2</td>
</tr>
<tr>
<td>$Ba_{0.90}Sr_{0.10}TiO_3$</td>
<td>3.978</td>
<td>3.998</td>
<td>15.5</td>
</tr>
<tr>
<td>$Ba_{0.85}Sr_{0.15}TiO_3$</td>
<td>3.971</td>
<td>3.987</td>
<td>8.4</td>
</tr>
<tr>
<td>$Ba_{0.80}Sr_{0.20}TiO_3$</td>
<td>3.970</td>
<td>3.980</td>
<td>3.6</td>
</tr>
<tr>
<td>$Ba_{0.70}Sr_{0.30}TiO_3$</td>
<td>3.69</td>
<td>3.699</td>
<td>1.2</td>
</tr>
</tbody>
</table>

3.7 MICROHARDNESS STUDIES

Hardness is one of the important solid state properties which determines the mechanical strength of materials (Wooster 1953). Hardness property is indicative of plasticity of the crystals. Hardness testing technique involves pressing a hard indenter into a sample surface and measuring the area of the resulting indentation. A diamond indenter is made to press the crystal surface by putting some load for a specific interval of time, during which plastic flow occurs, resulting in the formation of a permanent indentation.

BST single crystals with 10 and 20 mol.% of Sr were subjected to hardness test using a Leitz Wetzlar hardness tester fitted with a Vicker's diamond pyramidal indenter. Loads of 25, 50 and 100 g were applied over a fixed interval of time. Diagonal lengths ($d$) of the indentation were measured using a micrometer eyepiece. The Vicker's index is calculated using the expression
Figure 3.15  Hardness Vs Load for different mol.% of Sr for BST crystals
\( H_v = 1.8544 \frac{P}{d^2} \)

Here \( H_v \) is the Vicker's hardness number in Kg/mm\(^2\), \( P \) is the applied load in g and \( d \) is the average diagonal length in \( \mu \)m. Figure 3.15 shows the \( P \) Vs \( H_v \) for BST crystals with 10 and 20 mol.% of Sr. On increasing the load the hardness value decreases and at 100 g the hardness reaches a minimum value for both the compositions. When the load is increased above 100g, cracking starts. The decrease in hardness while increasing Sr concentration may be due to the decrease in bond energy.

3.8 CONCLUSION

Bulk twin free single crystals of barium strontium titanate with different concentrations of Sr have been grown. Sr incorporation eliminated the twin formation by inhibiting the hexagonal phase and increasing the stacking fault energy. Sr substitution favours the layer growth mechanism and hence the two dimensional nucleation. Single crystal X-ray diffraction studies confirmed the good quality of the crystal and it is found that the cell volume decreases on Sr doping. Laue and powder X-ray diffraction studies confirmed the single crystallinity and structure of the grown crystals. It is found that the system shifts to cubic phase for 30 mol.% of Sr. 90° c-domains have been observed and the twin angle has been calculated and compared with lattice parameters. The spontaneous polarization values decrease on increasing the Sr concentration. The phase transition becomes diffusive and the Curie temperature is reduced. For 30 mol.% of Sr, the Curie point falls below room temperature. Hardness value decreases on increasing the load and also Sr concentration.