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# Structural, dielectric and electrical properties of homovalent doped $SrSn_{1-x}Ti_xO_3$ $(0 \leq x \leq 0.08)$ system

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## Supplementary File

Fig S1 shows the X-ray diffraction pattern of all the samples. All the diffraction peaks are sharp and belongs to the crystal structure orthorhombic under space group *Pbnm* reported in theoretical database COD-1533387 for $SrSnO_3$[1].

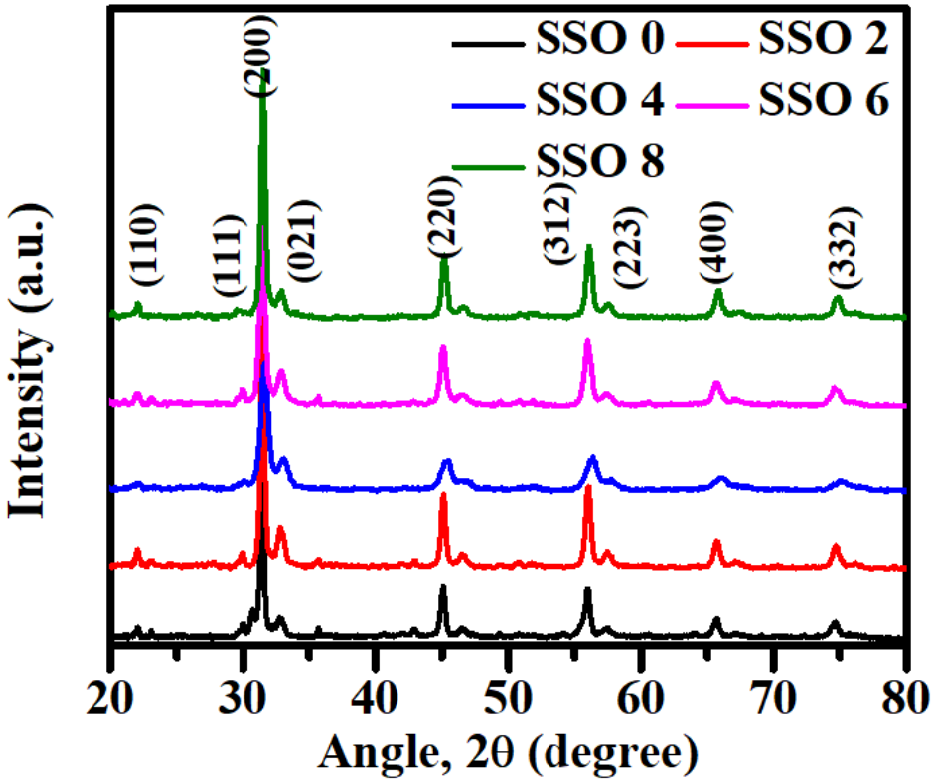


Fig S1 — X-ray diffraction pattern of obtained samples.

The Rietveld refinement performed on XRD data further reconfirmed the crystallization of samples in orthorhombic structure under space group *Pbnm*. The quality of fitting has been judged by calculating parameter $S$ using formula $R_{wp}/R_p$ (where $R_{wp}$ is weighted pattern profile parameter, $R_p$ is pattern profile parameter)[2]. The relevant parameters obtained from Riveted refinement are given in Table S1.

**Table S1 —** Lattice parameters, Volume, Angle, Refinement parameters, Bond length, Bond angle, Crystallite size, micro-strain of all samples.

| Parameters | SSO0 | SSO2 | SSO4 | SSO6 | SSO8 |
|---|---|---|---|---|---|
| **Structural parameters** | | | | | |
| a (Å) | 5.678 | 5.680 | 5.663 | 5.663 | 5.660 |
| b (Å) | 5.684 | 5.682 | 5.692 | 5.692 | 5.662 |
| c (Å) | 8.059 | 8.020 | 8.029 | 8.031 | 7.968 |
| Volume ($Å^3$) | 260.01 | 258.92 | 258.84 | 258.83 | 255.35 |
| X-ray density ($gm/cm^3$) | 6.44 | 6.25 | 6.18 | 6.17 | 6.15 |
| $\alpha = \beta = \gamma$ | 90 | 90 | 90 | 90 | 90 |
| **Rietveld refinement parameter** | | | | | |
| $R_p$ | 3.52 | 2.11 | 1.817 | 1.652 | 1.43 |
| $R_{wp}$ | 4.26 | 3.73 | 1.79 | 1.44 | 1.69 |
| $R_e$ | 4.12 | 3.51 | 1.48 | 1.14 | 1.23 |
| $S= R_{wp}/R_e$ | 1.03 | 1.06 | 1.20 | 1.26 | 1.37 |
| $\chi^2$ | 2.55 | 2.2 | 1.68 | 1.63 | 1.32 |
| **Bond length (Å)** | | | | | |
| Sr-O | 2.9443 | 2.7990 | 2.7989 | 2.7850 | 2.4840 |
| Ti/Sn-O | 2.0512 | 2.0436 | 2.0434 | 2.0411 | 2.0290 |
| Sr-Sn | 3.4600 | 3.4720 | 3.4717 | 3.4940 | 3.5420 |
| **Bond angle ($^0$)** | | | | | |
| O1-Ti/Sn-O1 | 180 | 180 | 180 | 180 | 180 |
| O2-Ti/Sn-O1 | 90.067 | 90.20 | 89.80 | 89.88 | 89.8819 |
| **W-H plot** | | | | | |
| Crystallite size (nm) | 48.46 | 36.09 | 34.22 | 33.31 | 28.86 |
| Micro-strain (x $10^{-3}$) | 1.36 | 1.45 | 2.04 | 2.45 | 2.86 |

## Determination of crystallite size and Micro-strain

Presence of definite width in the XRD peaks of sample ascribed to the smaller crystallite size, micro-strain, instrumental broadening, etc. Since the width of diffraction peaks initially corrected by recording the XRD pattern of Si-single crystal. Further, the contribution of crystalline size and micro-strain present in XRD peaks has been extracted using a well-known relation Williamson-Hall (W-H) plot. According to W-H plot, the total width of XRD peak can be written as the sum of the contribution arises due to smaller crystallite size ($\beta_D$) and due to micro-strain ($\beta_\epsilon$)[3].

$$\beta = \beta_D + \beta_\epsilon \qquad \text{S1)}$$

The value of $\beta_D$ from Debye equation, and $\beta_\epsilon$ as $4\epsilon \tan\theta$ were putting in equation (S1) and found to be;

$$\beta = \frac{0.9\lambda}{D\text{Cos}\theta} + 4\epsilon \tan\theta \qquad \text{(S2)}$$

$$\beta\text{Cos}\theta = \frac{0.9\lambda}{D} + 4\epsilon \text{Sin}\,\theta \qquad \text{(S3)}$$

The W-H plot for all the samples are generated using equation (S3) and shown in Figure S2. A linear equation ($y = mx + c$; $y = \beta\text{Cos}\theta, x = 4\,\text{Sin}\,\theta$) has been fitted to the experimental data to obtain the crystallite size and micro-strain. The slope of straight line gives micro-strain whereas intercept on y-axis is $\frac{0.9\lambda}{D}$ is used to determine the crystallite size. The value of crystallite size and micro-strain of all the samples are given in Table S1.

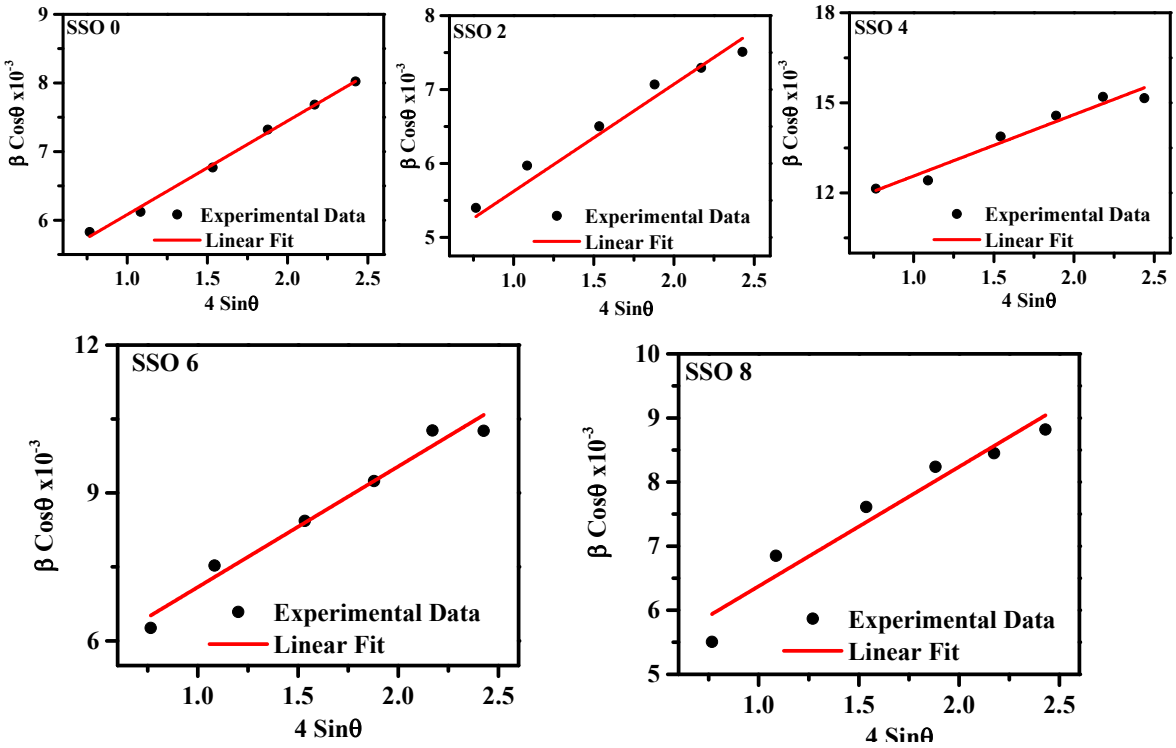


Fig S2 — W-H plot generated using equation S (3) for all samples.

It has been noticed from Table S1 that the value of crystallite size decreases, whereas micro-strain increases with increasing Ti in the lattice. The variation observed in crystallite size can be directly correlated with the ionic radii of $Ti^{4+}$ (0.605 Å) than $Sn^{4+}$ (0.69 Å)[4]. However, as Ti occupied the Sn-site it gives instability to structure and to prevent this instability a micro-strain arised in crystal structure. Thus, the value of micro-strain also increased as Ti increases in the lattice.

## References

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