Supplementary Information

Supplementary Information for:

Wide Range Bandgap Modulation in Strained $SrSnO_3$ Epitaxial Films

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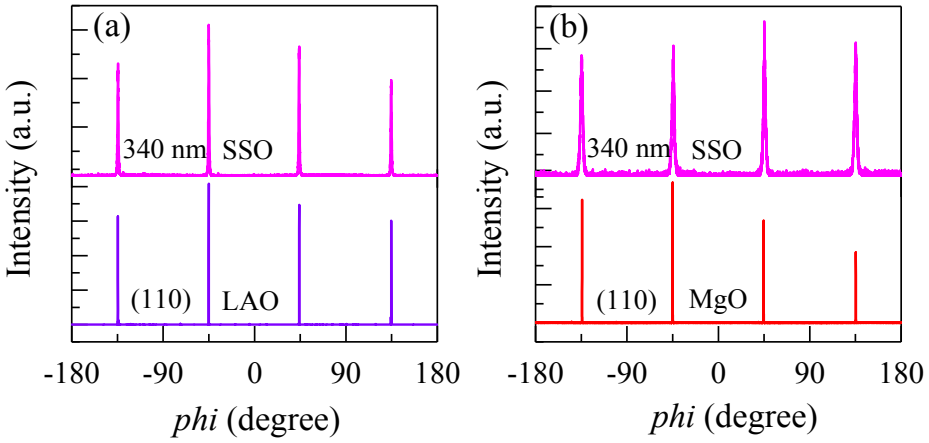

Fig. S1 The *phi* scans were measured around (110) SSO film (340 nm) and LAO, MgO substrates to reveal the epitaxial relationship between films and substrates and the results show that the films are epitaxially grown on LAO and MgO substrates with cubic-on-cubic epitaxial characteristics.

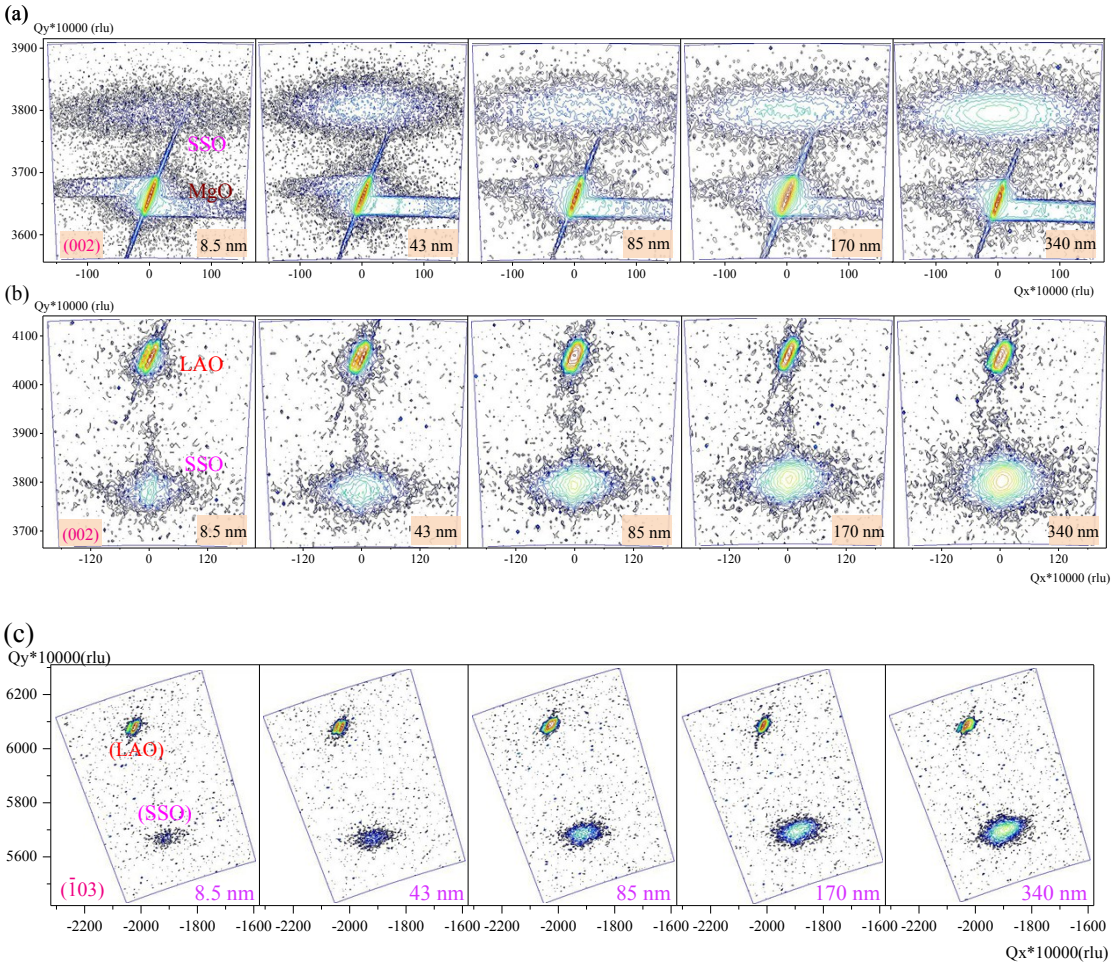

Fig. S2 The information of films strain states and lattice parameters of SSO films was obtained by performing RSMs around symmetric (002) and asymmetric (03) reflections of SSO films and LAO and MgO substrates. Due to the poor crystallinity of SSO films grown on MgO substrates, the information of films strain states around symmetric (002) reflections could not be provided here. The RSMs obtained from symmetric (002) reflections of SSO films grown on MgO and LAO substrates and from asymmetric (03) reflections with thickness of 8.5-340 nm. It can be concluded that these reflection spots are coming from the (002) SSO, LAO and MgO and (03) SSO and LAO. The out-of-plane and in-plane lattice parameters can be calculated from the spots positions using $c=3\lambda/2Q_y^*$ and $a=b=-\lambda/2Q_x^*$ (Q_y^* and Q_x^* are vertical and horizontal coordinates of the reciprocal space). With the increase of films thickness, the distance of two spots in each figure has slightly changes, indicating the strain gradually relaxed.

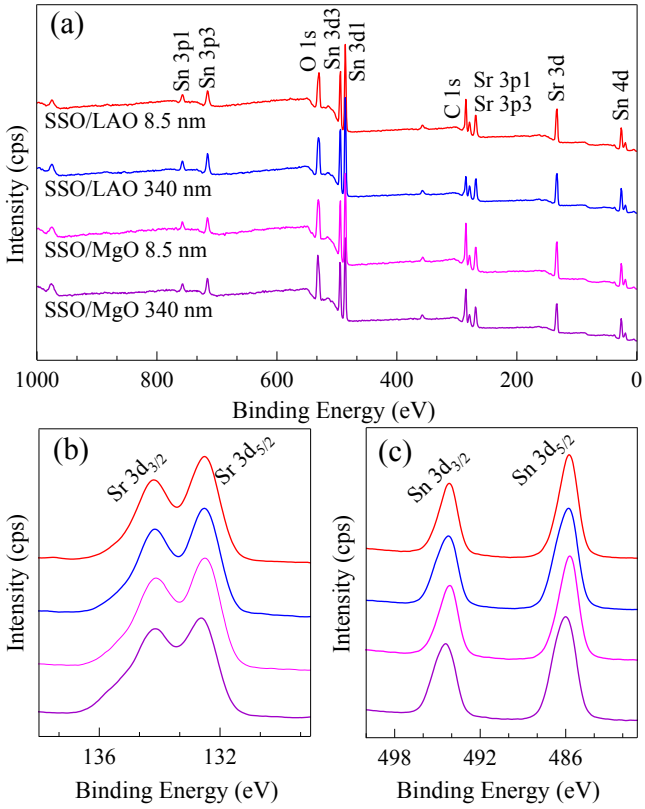

Fig. S3 (a) X-ray photoelectron spectra survey scans of the SSO thin films grown on LAO and MgO substrates with thickness of 8.5 and 340 nm, respectively. Narrow X-ray photoelectron spectra scan of (b) Sr 3*d*, (c) Sn 3*d*, respectively.

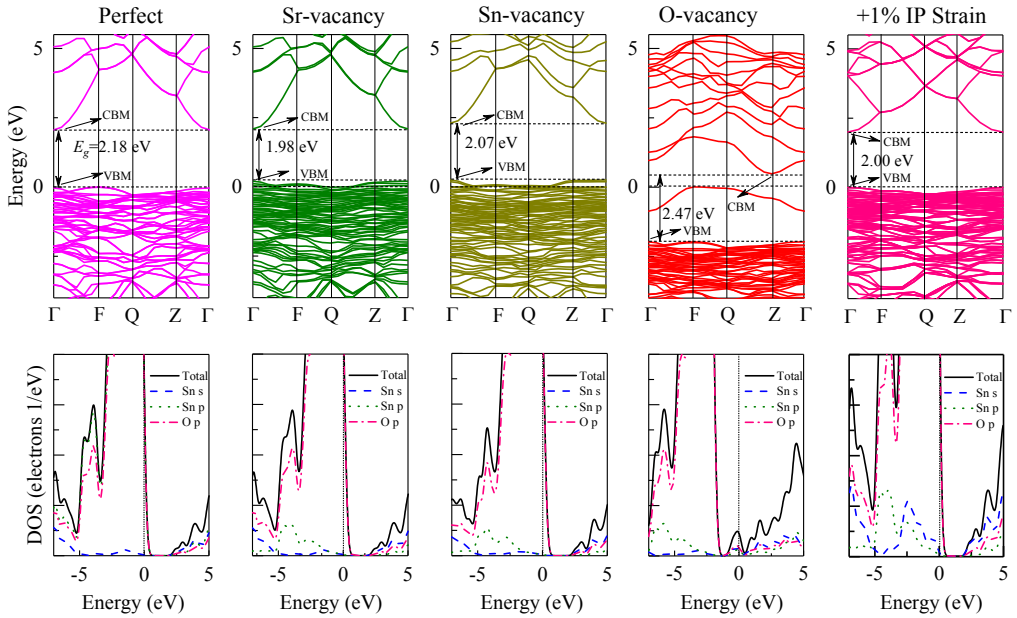

Fig. S4 To determine what cation-anion vacancy is likely to form, we calculated band structures (top) and total/atom resolved density of states (bottom) of 2×2×1 supercell of $SrSnO_3$ with perfect, Sr-vacancy, Sn-vacancy and O-vacancy model. And also we calculated the band structure of SSO under 1% IP tensile strain without VOs. The Fermi level is set at zero. The results showed that SSO with Sr and Sn-vacancy and under 1% IP tensile strain without VOs are not the reason for widening the band gap even lower it, which is due to the Fermi level lies in the valance band and CBM shifts to Fermi level, respectively. Oppositely, O-vacancy has significant effects on widening the band gap. Thus, we convinced that O-vacancy is easy to be formed in $SrSnO_3$ films under IP tensile strains.

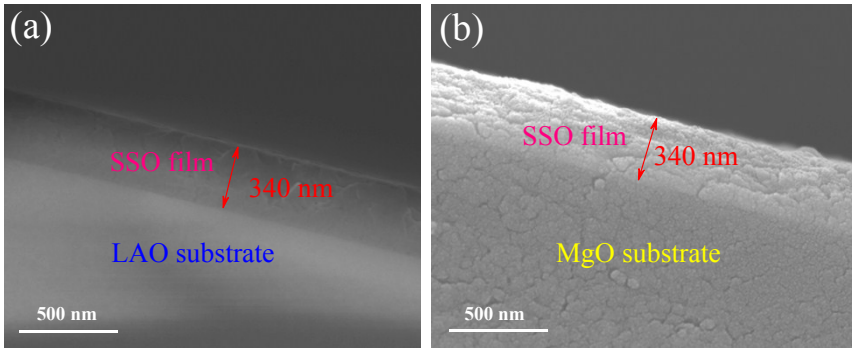

Fig. S5 The cross-sectional SEM image of a fracture surface of SSO films with a thickness of 340 nm grown on LAO and MgO substrates, respectively.