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Probing Electronic Structure of Co-Doped Srsno3 Using X-Ray Absorption near Edge Spectroscopy and Photoemission

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Extended Abstract

This study focuses on the exploration of La/Sb co-doped $SrSnO_3$ thin films as potential transparent conducting oxide (TCO) materials. TCOs are materials that possess both high electrical conductivity and optical transparency, making them suitable for various optoelectronic applications [1-3]. Traditional TCO materials based on binary oxides have been extensively studied, but recent research efforts have been directed towards perovskite-structured TCO materials due to their versatile structure and potential for enhancing the efficiency of perovskite solar cells. In this study, the electronic structure of La/Sb co-doped $SrSnO_3$ thin films prepared using the pulsed laser deposition (PLD) method was investigated. The La doping level is kept constant at 7% on the Sr site, while the Sb doping level varies from 0 to 3%. The resulting thin films exhibit high carrier mobility and optical transparency. To understand the changes in the conduction bandwidth and bandgap, the researchers employ X-ray absorption near-edge spectroscopy (XANES) and valence band spectroscopy (VBS) techniques. The XRD patterns confirm the orthorhombic-Pbnm structure of $SrSnO_3$, and the absence of impurity peaks indicates successful incorporation of La and Sb dopants into the lattice [4-5]. The XPS analysis reveals the presence of oxygen vacancies in the thin films, induced by both La and Sb doping. The oxygen vacancies contribute to the total electron concentration and are known to modify the properties of TCO materials. The Sn 3*d* spectra show the co-existence of Sn4+ and Sn2+ charge states, with Sb doping leading to an increase in Sn^{2+} content. The reduction of Sn^{4+} to Sn^{2+} is necessary to maintain charge neutrality and is attributed to the extra electrons generated by dopants and oxygen vacancies [6]. XANES spectra indicate a shift in the absorption edge with Sb doping, suggesting an increase in the conduction bandwidth and a decrease in the bandgap of the thin films. The combination of VBS and XAS spectra provides further insights into the electronic structure, showing an enhancement in O 2*p*-Sn 5*s* hybridization strength and a shift of the Fermi level towards the conduction band minimum (CBM) with Sb doping. The bandgap values obtained from VBS measurements support the reduction in bandgap with Sb doping. Overall, the La/Sb co-doped $SrSnO_3$ thin films exhibit desirable properties for TCO applications, including high carrier mobility and optical transparency. The study highlights the potential of co-doping strategies to improve the physical properties of TCO materials. The results also emphasize the influence of dopant site and species on the properties of TCO thin films. The findings contribute to the understanding of bandgap tuning and the role of oxygen vacancies in TCO materials. Further research in this direction may lead to the development of more efficient and versatile TCO materials for specific applications in optoelectronics:

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