BARIUM STANATE: PI-MOCVD THIN FILM DEPOSITION AND NONSTOICHIOMETRY ISSUES

Tomas Murauskas[1], Valentina Plaušinaitienė[1], Virgaudas Kubilius[1]

[1] Department of Inorganic Chemistry, Vilnius University, Lithuania
tomas.murauskas@chf.vu.lt

Cost-effective transparent conductive oxide (TCO) material composed of cheap and abundant elements is highly desired in nowadays optoelectronics. Recently a wide-bandgap La-doped barium stannate (LBSO) n-type semiconductor has been discovered. LBSO single crystal conductive properties rival those of Sn-doped In_2O_3 (ITO)[1]. Additionally, $BaSnO_3$ is of perovskite type lattice which allowing this material to be incorporated in various heterostructures as a lattice-matched electrode[2]. Although, achieving desirable thin film properties for optoelectronic applications is still challenging due to nonstoichiometry and various defects as well as substrate-films interaction – understanding of these factors is crucial for BSO applications. Therefore, in this work thin undoped $BaSnO_3$ films have been deposited using pulsed injection metal organic chemical vapor deposition (PI-MOCVD) method allowing easier compositional control and simultaneous deposition on multiple substrates. In order to achieve low and high film/substrate lattice mismatch, pseudocubic $LaAlO_3$, $SrTiO_3$ and hexagonal Al_2O_3 substrates were selected respectively. $Sn(thd)_2$ and $Ba(thd)_2$ precursor solution with various ratios in dimethoxyethane was used for thin film deposition. Depositions were carried out in $Ar:O_2$ (8:2 v/v) atmosphere. Layer composition was determined using ICP-MS and Energy Dispersive X-ray (EDX) spectroscopy techniques. Surface morphology and film structure were characterized using Scanning Electron Microscopy (SEM) and X-ray diffractometry. Optical properties were investigated using variable angle spectroscopic ellipsometry and UV-Vis spectrophotometry in transmission mode.

Thin BSO films deposited on (100) $LaAlO_3$, (100) $SrTiO_3$ substrates were highly epitaxial. While polycrystalline films were obtained on Sapphire C substrate. It was determined that a surplus amount of $Ba(thd)_2$ is required to produce stoichiometric films. Interestingly, slight deviation form stoichiometric ratio resulted in significant structural and optical changes while a cubic symmetry was maintained. Also, no additional phases were detected even with a drastic increase of Ba/Sn ratio. Strong lattice parameter correlation with the Ba/Sn ratio in the films suggests a defect-forming mechanism related to oxygen, barium atom vacancies and $(BaO)_2$ Ruddlesden-Popper crystallographic shear faults.

[1] Hanjong Paik, Zhen Chen et al., Adsorption-controlled growth of La-doped $BaSnO_3$ by molecular-beam epitaxy, APL Materials, **5**, 116107 (2017).

[2] Useong Kim, Chulkwon Park et al., All-perovskite transparent high mobility field effect using epitaxial $BaSnO_3$ and $LaInO_3$, APL Materials **, 3**, 036101 (2015).