Microstructure – properties relationship in new Zn-IV-N_2 thin films for photovoltaics applications

Prof. Jean-François PIERSON

Institut Jean Lamour (UMR CNRS 7198), University of Lorraine, Nancy, France

Zn-IV-N_2 (IV = Sn or Ge) semiconductors are promising optoelectronic materials and good candidates for thin film photovoltaic absorbers. Due to their tunable band gap (1.4-3.2 eV) and the choice of earth-abundant and non-toxic elements, they may replace $In_xGa_{1-x}N$ alloys materials commonly used for optoelectronics devices. Recently, few works investigate the disorder caused by unintentional oxygen incorporation, and the grains boundaries oxygen contamination in $ZnSnN_2$ thin films. To reduce oxygen contamination and improve physico-chemical properties, a new approach is investigated by the use of bias during film growth.

This work shows the results of $ZnSnN_2$ thin films grown by reactive co-sputtering using zinc and tin metallic targets in a nitrogen reactive atmosphere. The stoichiometry control of the film composition was managed by optimizing the target currents and the nitrogen partial pressure. The composition was measured by electron probe microanalysis (EPMA) to study the evolution of oxygen content under bias conditions. The application of different bias powers (from 0 to 50 W) modified the morphology and the composition of the films by densifying and decreasing significantly the oxygen contamination from 6.7 to 2.0 at. %. The optical band gap has been deduced from UV-visible spectroscopy and electrical properties was investigated by I-V experiments and Hall effect measurements. Ab initio calculations estimate an optical band gap in the order of 1.37 eV (calculated with a hybrid functional mBJ), the practical use of this system has been limited because of the difficulty to reach expected value. Here, we demonstrate that the optical band gap energy can be decreased (from 1.7 to 1.34 eV) to the range of the predicted one by using bias magnetron sputtering at room temperature. UV-visible spectroscopy highlights the reduction of the absorption by free electrons in the IR range responsible for the Burstein-Moss effect. Using first principle calculations, we explore the electronic structure and optical properties to compare with experimental results and we observe a good agreement. The study of bias effect power from 0 to 50 W underlines that an optimal parameter of 20 W bias is a compromise to gain the best structural, electrical and optical properties. Our results provide an interesting method to obtain a potential candidate for photovoltaic application, in an environmental friendly way, for a low-cost industrialization.

Keywords: photovoltaic, $ZnSnN_2$, bias effect, thin films, magnetron co-sputtering.