

An experimental and theoretical study on the physical properties of Al doped ZnO thin films

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Abstract: In this research, ZnO thin films with Al impurity as dopant were coated onto cleaned glass substrates by the spray pyrolysis technique. Crystal structure of the thin films was studied via XRD, and UV-vis spectroscopy was carried out to investigate their optical properties. Finally, in order to study the effect of Al impurity in ZnO thin films, the band structures of both pure and doped systems were calculated and compared using ab initio calculations in the frame work of DFT. The results show that polycrystalline thin films with hexagonal wurtzite structure have been grown, and the crystal size of the (002) ones is 25.41 nm. Moreover, the transmission in the visible region is more than 80%. Furthermore, Fermi energy is shifted into the conduction band in the case of Al doped ZnO which leads to increasing the electrical conductivity and changing the optical transmission threshold.

Keywords: zinc oxide; spray pyrolysis; Al impurity; density functional theory.

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