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Influence of hydrogen incorporation associated to thermal treatments on the optical and electrical properties of Al-doped ZnO thin films.

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Doped ZnO is considered a promising transparent conductive oxide (TCO) for advanced technological applications. So far, elements from III group (Al,Ga) proved to be suitable dopants to increase both electrical and optical properties of ZnO. On the other hand, the realization that hydrogen itself can act as an electrically active impurity in ZnO opened new routes towards the production of TCOs with adequate performances. In fact, hydrogen incorporation in the oxide structure during film growth or by post-treatments may result beneficial to further improve the optical and electrical quality of n-type semiconductors, even in presence of other extrinsic dopants. In this work we studied the effect of post-deposition annealing in Ar:H2 atmospheres on the properties of Al-doped ZnO (AZO) thin films. AZO thin films were deposited by RF sputtering in pure Ar discharges using a ceramic target containing 98 wt.% ZnO and 2 wt.% Al2O3. The films were sputtered at room temperature as well as at high temperature (Tsubstrate>250°C) then annealed in Ar and Ar:H2 atmospheres in a temperature range of 250-550°C, reaching resistivity values as low as 1E-3 Ωcm, carrier density values of 5.2E+20cm-3, mobility values of 10 cm2/Vs, while maintaining excellent transparency levels in the visible range (average T>82%). A full characterization of the films chemical, structural and optical properties by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and UV-visible spectrophotometry and of their electrical characteristics by Van der Paw and Hall effect measurements allowed to get insights on the role of hydrogen in improving films quality. We observed that hydrogen rich atmospheres during post processing thermal treatments have a synergic effect on the doping of the oxide matrix, by introducing free carriers into defect energy levels near the bottom of the conduction band which results in a significant increment (+7%) of the optical band gap.

Keywords
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