Investigation of structural, optical and electrical properties of (Li/Cu,N):ZnO codoped thin films

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Abstract

The effect of (Li/Cu, N) codoping on the properties of ZnO thin films are examined in view of their possible applications as p-type ZnO in transparent electronics, optoelectronic devices, ultraviolet light emitters or spin electronics [1-3]. Thus, the structural, optical and electrical conduction properties of the films synthesized by sol-gel method were investigated by field emission scanning electron microscopy (FESEM), x-ray diffraction (XRD), transmission and absorption (T/A), photoluminescence (PL) and I-V measurements in order to bring evidence on acceptor centers formation by dual-acceptor codoping processes. The (Li 3%,N 5%):ZnO films consist of crystallites with average size of 15 nm, show 95% transmission in the visible region, and an optical band gap of 3.22 eV. The PL spectra show emission maxima at 3.21 eV and 2.96 eV which are related to acceptor centers emission and the presence of defects, respectively. Li occupies interstitial sites and may form Li_i-N(O) defect complexes that act as acceptor centers. The (Cu 3%,N 5%):ZnO films consist of crystallites with average size of 12 nm, exhibit 90% transmission in the visible region. The PL spectra reveal band edge emission at 3.23 eV and defect related emission at 2.74 eV. In the (Cu,N) codoped films copper substitutes zinc and adopts mainly the Cu^{1+} state. We suggest that a defect complex involving Cu-N(-Zn_i-V_O) may determine the transition from n- to p-type conductivity. The discussion of these findings with reference to results of electronic band structure calculations on simple models brings new insights into defect formation mechanisms in the investigated films.

[1] Lyons J L, Janotti A, Van de Walle C G *2014 J. Appl. Phys.***115** *012014.*
[2] Plugaru R, Danciu A, Mihalache I, Plugaru N *2014 Electroceramics XIV Conference, Bucharest Romania 15th-20th June Conference Abstract book 180. http://www.electroceramics14.com/abstractbook.php*
[3] Plugaru R, Danciu A, Danila M, Plugaru N *2014 CMSE Conference, Shanghai China, 20th-23rd October Conference Proceedings of Abstract 8. http://www.cmseconf.org/2014/files/Proceedings%20of%20Abtract.pdf*