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Al in ZnO - An investigation of Al electrical activation in relation to structure and charge transport limits

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The search for a cost-effective alternative material to Sn doped In_2O_3 oxide has stimulated substantial research efforts in the field of ZnO based transparent conductive oxide (TCO) thin films. An important question relevant for fundamental research as well as practical applications is to which extent the charge transport properties of TCO materials can be ultimately improved. Considering that the ionized extrinsic donor impurities (Al) deliberately introduced into the ZnO host lattice in order to increase the electron density also generally dominate the charge carrier transport, it seems plausible that a certain limit exists where further extrinsic doping results in diminishing returns in resistivity, i.e. the gain in electron density is compensated by a loss of electron mobility. Therefore, it is attractive to decrease the Al concentration to a minimum while achieving as high as possible electrical activation, However, despite intense research related to ZnO, systematic and reliable quantitative experimental studies of Al electrical activation are rarely found in literature.Therefore, in this study, the effective electrical activation of Al in ZnO thin films grown by pulsed reactive magnetron sputtering is quantified experimentally for a wide range of Al concentrations [1]. We find that the activation does not exceed 35% remaining constant for growth temperatures below a certain optimum value at which the highest free electron density and mobility are achieved. Above this temperature, the Al activation decreases rapidly, while Al is accumulating in the films and their micro-structure as well as electrical properties deteriorate significantly. The analysis of possible mechanisms of Al deactivation suggests that the observed effects may be explained only by considering Al doped ZnO as metastable solid solution showing a tendency to segregation of Al into secondary phases.
[1] S. Cornelius and M. Vinnichenko, TSF 2015, http://dx.doi.org/10.1016/j.tsf.2015.11.059

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