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# Nitrogen doped ZnO films deposited by reactive RF magnetron sputtering

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Development of efficient optical blue and UV optoelectronic devices based on ZnO has been hindered by dificulties in obtaining films with controlled and stable p-type conductivity. In attempting to obtain reliable *p*-type doping of ZnO, the main effort has been directed on group VA elements, mainly nitrogen (N), which generate acceptor states when incorporated substitutionally at O sites. In this contribution we have investigated the characteristics of N doped ZnO thin films deposited on c-sapphire and glass by RF-magnetron sputtering at different temperatures,using a ZnO target in an ($Ar+O_2+N_2$) atmospherekept constant (0.5 Pa); N doping was varied by modifying $N_2$ flow. The films exhibited a wurtzite structure -preferred orientation (002). The films were analysed by AES and XPS. Hall,optical transmission/absorption and Raman measurements were also done. We have also carried out a DFT study of the localization,structure and occupation of the states induced by N doping in bulk wurtzite-type ZnO and thin films. Supercell calculations have been performed assuming a random and isolated N impurity substitutional distribution at O sites in the concentration range up to 11.12 at. %.We have used the FPLO9 code with L(S)DA and GGA functionals for the treatment of exchange and correlation potential. The density of states (DOS) of the bulk doped systems show a LDA band gap of 1.45 eV and that the nitrogen 2p states are located just above the top of the valence band crossing the Fermi level. The characteristics of the defect states observed in the DOS of bulk and thin films is discussed with reference to the experimental optical results.

**Keywords**
ZnO films
N doping
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