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**Theoretical simulation of doping mechanisms in p-type ZnO**

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— The efficiency of doping in crystalline semiconductors is related to the high concentrations of a certain type of defects. We have developed a universal approach to relate the concentrations of desirable defects as a function of the doping process experimental parameters such as the growth temperature. As shown in our previous work (J. Appl. Phys. 105, 113711 (2009)) our calculations reproduce well the experimental results for the *p*-type doping of ZnO with Phosphorus prepared by RF Sputtering, PLD and MBE. For the *p*-type doping of ZnO, at least one supplementary complication arises as the oxygen vacancies created during the process greatly diminish the number of holes. For the case of *p*-type doping of ZnO by implantation with +1 charged P and As ions, we calculated the efficiency of doping, together with the extent of O vacancy contamination, for a range of substrate temperatures from 30 to 700 $^\circ$C. The results show that As gives raise to hole densities three orders of magnitude higher than P (therefore recommending As a more efficient *p*-type dopant than P) and that many O vacancies are created during the ion implantation process. The high density of O vacancies resulting from our calculations may explain the poor stability and reproducibility of *p*-type ZnO.

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