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Impact of Mg Content on (Mg,Zn)O Native Point Defects MOLLY BALL, OSCAR RESTREPO, LEONARD BRILLSON, WOLFGANG WINDL, The Ohio State University, DEPARTMENT OF MATERIAL SCIENCE AND ENGINEERING COLLABORATION, DEPARTMENT OF PHYSICS COLLABORATION — The two most thermodynamically stable defects in ZnO are oxygen vacancies (V_O) and zinc vacancies (V_{Zn}). These native point defects are electrically charged and can contribute to free carrier densities. Experiment shows that Mg addition to ZnO significantly changes native defect densities. To better understand this dramatic decrease in V_{Zn} and V_O-related defects with increasing Mg content up to x=0.44 and the subsequent increase, we performed density functional theory (DFT) calculations using PAW potentials within PBE using VASP. The results showed to be very sensitive to DFT method used and chemical-potential calculation. For the latter, the literature shows that one can assume that the oxygen chemical potential equals that of the atoms in the oxygen molecules at a given surrounding partial oxygen pressure. However, one can also postulate that the total defect concentrations conserve the stoichiometry, or limiting potentials from elemental equilibrium phases can be used. The experimentally observed dependence helped identify the correct way to reproduce the experimental dependence of formation energy on Mg concentration, which will be discussed in detail in this presentation.

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