Defect Distribution and Electronic Properties of the IrO_x/ZnO Interface

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We used depth-resolved cathodoluminescence spectroscopy (DRCLS) to measure the spatial distribution of native point defects at Zn- and O-polar ZnO interfaces with iridium oxide (IrO_x) and their impact on Schottky barrier formation. Oxidized metal, such as IrO_x and PtO_x, have sparked interest in their high work functions allowing them to be used as both Ohmic and Schottky contacts[1]. These oxidized metal layers produce Schottky contacts with the ZnO. These diodes have rectification of 8.6 and 5.5 orders of magnitude, respectively, with barrier heights of 0.89 eV and 0.67 eV. For the same RF sputter of a 32 nm IrO_x layer, on ZnO, sample on both Zn-polar and O-polar ZnO, incident electron beams with energies E_B = 1 -5 keV generated electron-hole (e-h) pairs that recombined to exhibit DRCLS spectra past the IrO_x layer, with 3.35 eV intrinsic band gap transitions in ZnO, and 2.01 eV and 2.08 eV V_{Zn} transitions in the Zn-polar and O-polar ZnO respectively. V_{Zn} acts as a compensating defect, acting to increase the depletion width at the IrO_x/ZnO interface creating the Schottky diode [2]. DRCLS enabled us to profile the V_{Zn} density across the IrO_x/ZnO interface on a near nm scale as defined by Monte Carlo simulations of electron-hole (e-h) pair creation rate vs. depth. This defect depth precision revealed interfaces with V_{Zn} profiles in the ZnO that varied with the Zn-Polar and O-polar ZnO orientations. The depth profiles show a clear difference in the density of V_{Zn} in each sample with nearly a 1.5 times increase in V_{Zn} density from the O-polar to the Zn-polar sample.

The variation of the V_{Zn} between each is significant since it explains the higher barrier height in the Zn-polar ZnO. This increased barrier height from growing oxidized metals on semiconductor films could have implications since these high work function metals could be used as Ohmic contacts on p-type semiconductors. The authors gratefully acknowledge support from National Science Foundation Grant No. DMR-1305193 (Charles Ying and HaiyanWang).

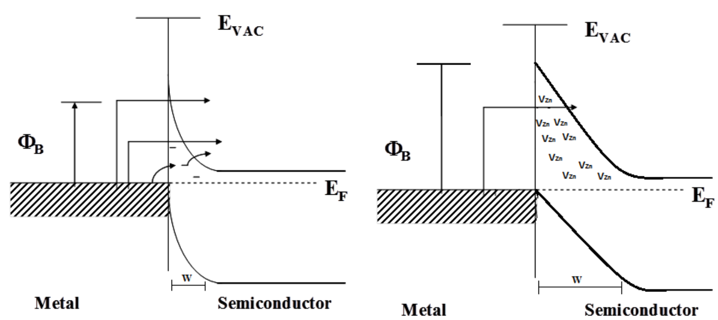

Figure 1: Band diagram showing a widening depletion region in the presence of the acceptor defect V_{Zn}.

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[1] G. T. Dang, T. Uchida, T. Kawaharamura, M. Furuta, A. R. Hyndman, R. Martinez, S. Fujita, R. J. Reeves, and M. W. Allen, "Silver oxide Schottky contacts and metal semiconductor field-effect transistors on SnO2 thin films," vol. 041101, 1882.
[2] Y. Dong, F. Tuomisto, B. G. Svensson, A. Y. Kuznetsov, and L. J. Brillson, "Vacancy defect and defect cluster energetics in ion-implanted ZnO," *Phys. Rev. B - Condens. Matter Mater. Phys.*, vol. 81, no. 8, pp. 3–6, 2010.