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Acceptors in bulk and nanoscale ZnO[1]

M.D. MCCLUSKEY, Washington State University

Zinc oxide (ZnO) is a semiconductor that emits bright UV light, with little wasted heat. This intrinsic feature makes it a promising material for energy-efficient white lighting, nano-lasers, and other optical applications. For devices to be competitive, however, it is necessary to develop reliable p-type doping. Although substitutional nitrogen has been considered as a potential p-type dopant for ZnO, theoretical and experimental work indicates that nitrogen is a deep acceptor and will not lead to p-type conductivity. This talk will highlight recent experiments on ZnO:N at low temperatures. A red/near-IR photoluminescence (PL) band is correlated with the presence of deep nitrogen acceptors. PL excitation (PLE) measurements show an absorption threshold of 2.26 eV, in good agreement with theory. Magnetic resonance experiments provide further evidence for this assignment. The results of these studies seem to rule out group-V elements as shallow acceptors in ZnO, contradicting numerous reports in the literature. If these acceptors do not work as advertised, is there a viable alternative? Optical studies on ZnO nanocrystals show some intriguing leads. At liquid-helium temperatures, a series of sharp IR absorption peaks arise from an unknown acceptor impurity. The data are consistent with a hydrogenic acceptor 0.46 eV above the valence band edge. While this binding energy is still too deep for many practical applications, it represents a significant improvement over the $\sim$ 1.3 eV binding energy for nitrogen acceptors. Nanocrystals present another twist. Due to their high surface-to-volume ratio, surface states are especially important. Specifically, electron-hole recombination at the surface give rises to a red luminescence band. From our PL and IR experiments, we have developed a "unified" model that attempts to explain acceptor and surface states in ZnO nanocrystals. This model could provide a useful framework for designing future nanoscale ZnO devices.

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