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Material and Optical Properties of ZnO-Based Alloys[1]

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ZnO is emerging as one of the materials of choice for UV applications. It has a relatively benign chemical nature, a deep excitonic energy level, and a direct bandgap of ~ 3.4 eV. The latter two properties make ZnO a highly efficient light-emitter at room and above room temperatures. Alloying ZnO with certain atomic constituents has the potential to add new optical and electronic functionalities to ZnO. This work will focus on two alloy systems of ZnO: one is Mg(x)Zn(1-x)O, and the other is ZnS(1-x)O(x). The x in the formula is the percent composition of the alloy constituents; upon changing the composition, the bandgap and the optical properties can be tailored from those of one end member to the other. At the low Mg composition range, the Mg(x)Zn(1-x)O alloy has the hexagonal wurtzite structure and a bandgap that is tunable in the range of ~ 3.4 (that of ZnO) up to approximately 4 eV. At the high composition range the alloy forms with the cubic NaCl structure, and importantly its bandgap shifts into the deep UV range up to 7.4 eV (that of MgO). Thus, Mg(x)Zn(1-x)O can provide an alloy system with bandgaps and bandedge photoluminescence spanning the range of 3.4 eV to 7.4 eV that are achieved via the choice of the composition x. However, due to the two different crystal structures of the end members, ZnO with the wurtzite and MgO with the cubic structure, at intermediate composition range the alloy is phase segregated. The other alloy system to be discussed is the ZnS(1-x)O(x). The bandgap of ZnO is 3.4 eV and that of ZnS is 3.8 eV; upon alloying ZnO with sulfur, the bandgap behavior exhibits a strong deviation from linearity due to the large difference in atomic size and chemical characteristics of the alloy constituents. Unlike Mg(x)Zn(1-x)O, the ZnS(1-x)O(x) is a highly lattice mismatched system that results in a strong bowing of its bandgap toward the visible range at the green-blue part of the spectrum. In this research, we present studies of the material and optical properties of both alloys. The issue of solubility and phase segregation studied via X-ray diffraction, photoluminescence, and atomic imaging, is addressed. The optical properties that were studied via absorption and photoluminescence are discussed. The optical properties studied include bandgap tailoring, the nature of the optical emission specifically exciton and defect photoluminescence, and the phonon dynamics of the alloys.

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