

Optical selection rules and scattering processes in rocksalt wide band gap ZnO

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Abstract

At sufficiently high pressures, wurtzite structure zinc oxide (W-ZnO) can be transformed to the cubic rocksalt (R-ZnO) structure. The R-ZnO exhibits semiconductor behavior with an indirect wide band gap of inline image. The maximum valence band is found far away from the center of the Brillouin zone (BZ) at high symmetry point L and line S, depending on the pressure. The unusual electronic band structure (EBS) of the R-ZnO leads to several direct and indirect optical transitions which find applications in ultraviolet optoelectronic devices. We have investigated radiative and non-radiative symmetry restricted selection rules, as well as inter- and intra-valley scattering processes.