Theory of Excitons in ZnO/ZnMgO Quantum Wells

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Literature reports on high quality ZnO/ZnMgO heterostructures opened new hopes for applications of theses materials for optoelectronic devices operating in the ultraviolet optical region and for and flexible electronics.Due to the large exciton binding energy and small effective Bohr radius pronounced excitonic features may be observed in the optical spectra in a very large range of quantum well widths even at room temperature.[1] Precise interpretation of the optical spectra is however hindered by the presence of built-in strain caused by the lattice mismatch with the substrate. Further ambiguity is introduced by the strong local electric field induced by the polarization charge density and the background doping.[2] Finally, the sp^3 hybridization of atomic orbitals in ZnO leads to the complicated structure of the conduction and valence bands. In particular the sequence of the valence band levels in the bulk ZnO, which is still a matter of controversy, may be strongly dependent on the built-in strain. In particular, taking into account the spin, the twofold conduction band level has Γ_7 symmetry while the sixfold top of the valence band is split by the crystal field and spin-orbit interaction into one twofold Γ_9 level and two Γ_7 levels. It is commonly believed that the topmost valence band level has Γ_9 symmetry although it was shown that in the regime of negative spin-orbit interaction, the sequence Γ_7 - Γ_9 - Γ_7 is also possible.[3] This ambiguity is related to the fact that the spin-orbit coupling in ZnO seems to be fairly small. The detailed model of the absorption spectra in the vicinity of the fundamental gap is therefore of fundamental importance in studying such systems. In this report we present a multiband exciton absorption model in ZnO/ZnMgO quantum wells which takes into account the details of the valence band structure. In our model we incorporate the **kp** coupling between valence subbands as well as the direct and exchange Coulomb interaction between the electron and hole [4]. The effect of the electric field is accounted for using proper potential profile of the quantum well while the built-in strain is incorporated via Rashba-Sheka-Pikus effective Hamiltonian. The Bethe-Salpeter equation for the two particle correlation function is solved in the basis of Landau orbitals corresponding to an optimized, fictitious magnetic field B directed along the QW growth axis. Using the Lanczos reduction procedure we obtain full absorption spectra from which the exciton binding energies and life-times may be deduced. The calculations are performed for the circular polarization of light (Faraday configuration). Our model may be useful in interpretation of experiments investigating the electronic structure near the fundamental gap of both ZnO and ZnMgO.

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