DFT simulation of the physical properties of AlN/GaN multiquantum well (MQWs) system

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Density functional theory simulations (DFT) were used to obtain physical properties of AlN/GaN multi-quantum wells (MQWs) systems. To overcome the Kohn-Sham band gap (BG) underestimation, we have applied a method proposed recently by Ferreira et al., called LDA-1/2 which approximately includes the self-energy of excitations in semiconductors, providing BG energies, effective masses, and band structures in very good agreement with experiment [1]. Systematic DFT studies were conducted to determine an influence of changing of the well/barrier width ratio on the properties of AlN/GaN MQW system such as the electric field, polarization charges and polarization dipoles within the well-barrier structure. It was shown that these fields depend critically on the well-barrier thickness ratio. A comparison of the fields proves that the DFT results recover basic trends predicted by the theory based on spontaneous and piezoelectric polarization, computed from the Berry-Phase approach in Ref. [2]. Generally, the fields obtained from the Poisson solution in the DFT calculations are greater than these predicted by the polarization models. We relate this error to the BG underestimation which was not corrected by the authors in the last reference. The field gives rise to Quantum Confined Stark Effect (QCSE), changing the energies of quantum states of the electrons and holes in the wells and also separating the wavefunctions of both quasiparticles in space. The overlap of these functions is calculated, showing considerable separation in space which significantly reduces the oscillator strength of the optical transitions, and consequently, the optical efficiency of nitride based light emitting diodes (LED) and laser diodes (LD), especially for wider structures. For wider barriers, the energies of the transition displays the crossover from narrow minima type where the parallel polarized transition has a lower energy to wide wells where the perpendicular polarized emission is lower in the energy scale. This is related to the crossover of the CH and LH/HH bands, as postulated in Refs [3, 4]. For the narrow GaN layers, the optical strength is higher for perpendicular polarized transitions which is in agreement with the experimental results in Ref. [5], where a stronger emission was observed for the c-axis direction. For wider wells, the strengths falls much faster for perpendicular polarization which indicates the important role of the band offsets. The results were also used for optaining a spatial distribution of the bands in structures with atomic resolution which allows direct estimation of the band offset.

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