Topological Quantum Phase Transition in InN/GaN Quantum Wells under Hydrostatic Pressure

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The topological insulator (TI) state is a state of matter characterized by a bulk excitation gap and topologically protected helical edge states with zero energy gap. Closing of the gap at the surface is caused by the nontrivial topology of the bulk characterized by nonzero topological invariants [1]. Recently, it was shown theoretically that in narrow InN/GaN quantum wells (QWs) grown along (0001) crystallographic direction of the wurtzite structure, the extremely large built-in electric field originating from piezoelectric effect and spontaneous polarization may close the energy gap and induce a considerable Rashba spin-orbit interaction leading to the possibility of the observation of the TI state in a Hall bar structure [2]. The built-in electric field is increased in InGaN/GaN QWs by hydrostatic pressure which reduces the pressure coefficient of the energy gap even to negative values [3]. Consequently, by applying hydrostatic pressure to narrow InN/GaN QWs, one may observe the energy gap closing and inversion of the conduction and valence bands. These conditions lead to a possibility of the pressure-induced phase transition from a ordinary (i.e., topologically trivial) semiconductor to the TI state.

In this work, we study theoretically the pressure-induced phase transition between normal and TI states in InN/GaN QWs in a stripe geometry. We use eight band k·p method to construct a two-dimensional six-band effective Hamiltonian, which takes into account the coupling between the conduction, light hole and heavy hole states. In order to describe correctly pressure evolution of strain and the built-in electric field entering the eight band k·p Hamiltonian, we use the nonlinear theory of elasticity and piezoelectricity including contributions arising from the second-order piezoelectric constants and the third-order elastic constants [4]. The effective Hamiltonian is used to calculate the electronic states in an infinite long Hall bar structure.

Band-structure calculations have been performed for 1.3 nm wide InN/GaN QWs with 40 nm thick barriers, grown on GaN substrate. The thickness of an infinite long Hall bar structure was equal to 100nm. At ambient pressure, the sequence of bands for this structure is normal, i.e., the conduction band is above the heavy hole and light hole bands, and the energy gap is equal to 93 meV. Applying hydrostatic pressure reduces the energy gap with the pressure coefficient equal to –9 meV/GPa and leads to the crossover between the conduction band and the heavy-hole band at 10.5 GPa. Interestingly, the helical edge states with a linear dispersion near the center of the Brillouin zone appear at about 11 GPa, when the conduction band inverts with the light-hole band.

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