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Symmetry-induced effects on the band structure of wurzite III–V nitride-based quantum wells

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Abstract. The symmetry of wurzite III–V nitride-based quantum wells (QW) is shown to be described by the layer group P3m1 (DG 69) and does not depend on the number of atomic monolayers constituing the QW. The modification of bulk electron state symmetries and optical transition selection rules when inserting a QW is established.

Introduction

The III–V nitrides (GaN, AlN, InN) and heterostructures based on these materials have been intensively studying during the last years both theoretically and experimentally [1]. The fast progress in MBE and MOCVD technologies allowed to fabricate heterostructures such as superlattices and quantum wells (QW's) with layer widths comparable with the GaN lattice constant [2].

Usualy, when studying QW's one speaks about two-dimensional (2D) systems that is not completely correct. Indeed, due to confinement, the carriers are allowed to move only in directions parallel to the layer, i.e. their $\mathbf{k}$-vectors have only $\mathbf{k}_x$ and $\mathbf{k}_y$ components and the corresponding Brillouin zone (BZ) is 2D. However, the electron wave functions are still 3D. The same is true also for lattice vibrations which can have atomic displacement components along all three directions. Next, when analyzing optical selection rules, the vector representation according to which the electric field is transformed should be taken also 3D. So, the system is still 3D though with 2D periodicity and needs a special symmetry description.

1. Layer symmetry of a single GaN/AlN QW

The insertion of a single GaN QW into the AlN bulk crystal destroys the translational symmetry along the direction perpendicular to the QW layer. (Below we choose this direction to be the sixfold rotational axis of the bulk crystal). The translational symmetry of such a system turns out to be 2D whereas the point symmetry remains 3D though can be different from that in the bulk crysal. The space group symmetry of the system is described by one of the 80 diperiodic groups in three dimensions which are called layer groups [3].

Thus, the Bravais lattice of the system (bulk AlN with a GaN QW) is 2D whereas the unit cell in the z-direction becomes an infinite column of atoms. However, though the system as a whole acquires layer symmetry, it is obvious from physical reasons, that beyond the QW region all the excitations are still "bulk-like" ones. Therefore, the layer symmetry determines mainly the excitations localized within the QW and adjacent parent crystal layers. Within the framework of symmetry, it is impossible to determine how many Al-N atomic planes adjacent to the QW one should take into account. However, it is possible

to understand how to separate the contribution of the QW spectrum from the bulk one basing on numerical calculations. In the bulk crystal, the number of degrees of freedom of the system (that determines the sets of electron states at each point of the BZ) equals to the number of atoms in the primitive cell multiplied by the number of localized orbitals per atom taken into account. For example, in the GaN bulk crystal there are 4 atoms per primitive cell (2Ga and 2N). If we take into account only s-, p_x-, p_y-, and p_z-orbitals then the number of degrees of freedom of the system will be 16. In this case, at the Γ point, s- and p_z-orbitals induce $4\Gamma_1 + 4\Gamma_4$ states (non-degenerate) whereas p_x- and p_y-orbitals induce $2\Gamma_5 + 2\Gamma_6$ states (doubly degenerate) [4]. When introducing a single QW, the number of degrees of freedom becomes infinite. If we begin with the minimal unit cell comprising only atomic planes of the QW and then add one Al-N monolayer from the adjancent layers we increase the number of electron states step-by-step. At last, new states added will not be differed from that of the bulk. Then one can say that the states obtained in the previous steps are originated from the QW.

We have determined that the symmetry of a single GaN QW in wurtzite AlN crystal does not depend on the number n of GaN monolayers constituing the QW. Its symmetry is described by P3m1 (DG 69) layer group with the atomic arrangement over the Wyckoff positions given in columns 1–3 of Table 1. However, there is a variation of occupation numbers of Wyckoff positions b and c with the same site symmetry which affects the sets of electron and phonon states at the BZ points other than Γ. Thus, the insertion of a QW results in lowering the point group symmetry from C_{6v} to C_{3v} since the sixfold screw axis is replaced by the threefold rotation one.

2. Electron state symmetry

The symmetry of electron states in the QW can be obtained by constructing the band representations of its layer group induced by those irreducible representations (irreps) of site symmetry group according to which localized Wannier-type atomic functions transform. The induced representations of a layer group DG can be obtained from the induced representations of the corresponding Fedorov space group G that can be expressed as a semi-direct product $G = T_3 \bigwedge DG$ where T_3 is a group of one-dimensional translations [5]. In the table of induced representations of the Fedorov group G one should take the lines corresponding to the Wyckoff positions of the diperiodic group DG, i.e., the positions having no coordinates expressed in fractions of translations along the z-axis. The 2D BZ of the DG is a section of the 3D BZ of the corresponding group G. The symmetry of electron states in the GaN/AlN QW obtained by the method of induced band representations [5] is given in Table 1. The irreps of the QW space group describing the symmetry of electron band states are generated by the single and double-valued (marked with a bar over an irrep symbol) irreps β of the groups $G_{\mathbf{q}}$ of the sites $\mathbf{q}$ where the atoms are located. The localized atomic orbitals of $s-$, $p-$, and d-types are transformed according to these site-group irreps. The space group irreps are labeled according to [6] and the labeling of site group irreps follows [7]. It is seen that the symmetry types of electron states at the BZ points do not depend on the dimensions of the QW unit cell. However, the number of times each irrep enters into each set of electron states does depend.

The QW can be considered as a limited case of a SL with infinitely large period and thin GaN regions. Thus, when increasing a SL period keeping the GaN region fixed, the SL BZ decreases in the $\mathbf{k}_z$ direction and transforms, at last, into a sheet being a cross-section of the bulk-crystal BZ. As a result, all the states from $\Gamma-A$, $K-H$, and $M-L$ symmetry lines will be projected into Γ, K, and M points, respectively.

Table 1. Electron state symmetries in GaN/AlN QW's (n is the number of Ga atomic planes in the QW, $m = 2s$ is the number of adjacent Al atomic planes at each side of the QW, N_I and N_{II} are nitrogen atoms in the QW and adjacent layers, respectively).

Atomic arrangement			$\mathbf{q}$	β	Γ	K	M
$n = 2s$	$n = 2k+1$				(000)	$\left(\frac{1}{3}\frac{1}{3}0\right)$	$\left(\frac{1}{2}00\right)$
	$n = 4s+1$	$n = 4s+3$			C_{3v}	C_3	C_s
$\frac{n}{2}$Ga	$\frac{n+1}{2}$Ga	$\frac{n-1}{2}$Ga	$1b$	$a_1(s; p_z)$	1	2	1
$\frac{n}{2}N_I$	$\frac{n-1}{2}N_I$	$\frac{n+1}{2}N_I$	$\left(\frac{1}{3}\frac{2}{3}z\right)$	$e(p_x, p_y)$	3	1,3	1,2
mAl	mAl	mAl	C_{3v}	$\bar{e}_1^{(1)}$	4	6	4
mN_{II}	mN_{II}	mN_{II}		$\bar{e}_1^{(2)}$	5	6	3
				$\bar{e}_2$	6	4,5	3,4
$\frac{n}{2}$Ga	$\frac{n-1}{2}$Ga	$\frac{n+1}{2}$Ga	$1c$	$a_1(s; p_z)$	1	3	1
$\frac{n}{2}N_I$	$\frac{n+1}{2}N_I$	$\frac{n-1}{2}N_I$	$\left(\frac{2}{3}\frac{1}{3}z\right)$	$e(p_x, p_y)$	3	1,2	1,2
mAl	mAl	mAl	C_{3v}	$\bar{e}_1^{(1)}$	4	4	4
mN_{II}	mN_{II}	mN_{II}		$\bar{e}_1^{(2)}$	5	4	3
				$\bar{e}_2$	6	5,6	3,4

The correspondence between the bulk and QW states is as follows:

$$\Gamma_{1,4}(A_{1,4}) \to \Gamma_1, \quad \Gamma_{5,6}(A_{5,6}) \to \Gamma_3, \quad \Gamma_{7,8}(A_{7,8}) \to \Gamma_6, \quad \Gamma_9(A_9) \to \Gamma_4 + \Gamma_5,$$
$$K_{1,2}(H_{1,2}) \to K_1, \quad K_3(H_3) \to K_2 + K_3, \quad K_{4,5}(H_{4,5}) \to K_5, \quad K_6(H_6) \to K_4 + K_6,$$
$$M_{1,4}(L_{1,4}) \to M_1, \quad M_{2,3}(L_{2,3}) \to M_2, \quad M_5(L_5) \to M_3 + M_4,$$

It is seen that the bulk states Γ_9, A_9, and M_5, L_5 split into complex-conjugated irrep pairs $\Gamma_4 + \Gamma_5$ and $M_3 + M_4$, respectively. These irreps form doubly-degenerate coreps and correspond to the same energy. The degeneracy is connected with time inversion and may be lifted when applying a magnetic field along the QW symmetry axis which does not modify the QW symmetry.

On the other hand, the states K_2 and K_3 (as well as K_4 and K_6) of the QW though described by complex-conjugated irreps do not form a corep and hence correspond to the states with different energies. This means that doubly-degenerate K_3 and K_6 bulk states split in the QW into pairs of states $K_2 + K_3$ and $K_4 + K_6$, respectively.

The correspondence between the conduction and valence band levels at the BZ centre of bulk GaN crystal and GaN/AlN QW as well as optical transitions involving these states are shown in Fig. 1. Note that, according to [8], the hierarchy of A,B,C exciton series in thin (less than 25 Å) QW's is different from that of the bulk. That is, in the QW, the A exciton formed by $\Gamma_4 + \Gamma_5$ level has higher energy than the B exciton formed by Γ_6 valence band level. It means that the $\Gamma_4 + \Gamma_5$ level originating from the uppermost valence-band level Γ_9 of the GaN bulk crystal is lower in energy than the Γ_6 level originating from the Γ_7 bulk level.

From Fig. 1, we see that in the QW the A, B and C exciton series obey the same selection rules as in bulk GaN [4]. The only difference is connected with A excitons. Since the A exciton is formed by the $\Gamma_4 + \Gamma_5$ corep, it splits when applying the magnetic field along the z-axis.

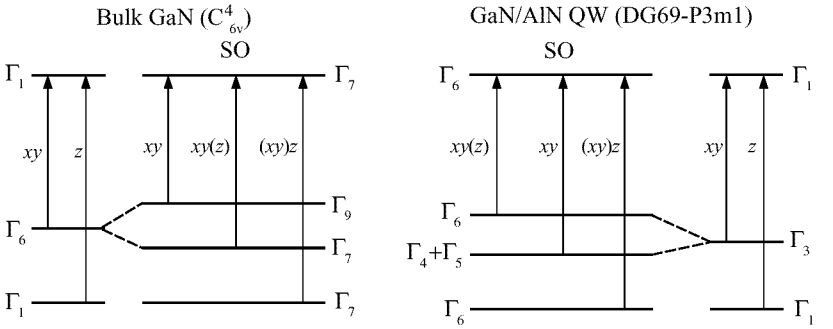

Fig. 1. Energy level diagrams at the BZ centre and allowed optical transitions for the GaN bulk crystal and GaN/AlN QW's. The allowed polarizations for the case when spin-orbit interaction is taken into account are shown in parentheses.

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