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Electron state symmetries and optical transitions in semiconductor superlattices: I. $(\text{GaAs})_m(\text{AlAs})_n$ grown along the [001] direction

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Abstract. Using the method of induced band representations of space groups, we have performed a complete group-theory analysis of electron state symmetries in $(\text{GaAs})_m(\text{AlAs})_n$ superlattices grown along the [001] direction. The spin-orbit interaction has been taken into account. The selection rules for both direct and phonon-assisted optical transitions have been derived. Using both the results of our group-theory analysis and data on the various electronic-structure calculations which have appeared in the literature, we predict some variations in the optical transitions when m and/or n are varied. We also propose optical experiments to decide among the numerous and sometimes contradictory results of those band calculations.

1. Introduction

The semiconductor superlattices (SLs) $(\text{GaAs})_m(\text{AlAs})_n[hkl]$ are a new class of artificially grown crystals whose structure (i.e. a space group G and an arrangement of atoms over the Wyckoff positions in a primitive cell) depends on the growth direction $[hkl]$ and numbers of monolayers (m , n) of constituent materials.

For each direction of growth, these SLs constitute several single-crystal families specified by different space groups G_1, G_2, \dots, G_r . By definition, within each family, the crystals have the same space group G_i but differ from each other by an arrangement of atoms over the Wyckoff positions. Thus, from the crystallographic point of view, the SLs with different numbers of monolayers m and n are distinct crystals, even those belonging to the same family.

Such a dependence of the SL crystal structure on the numbers of monolayers influences phonon and electron states in these crystals. The symmetry of phonon states and the corresponding infrared and Raman spectra selection rules have been investigated comprehensively for the $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs during recent years [1–5]. However, the symmetry of electron states and the corresponding optical selection rules in SLs have not been analysed in detail up to now.

To study the optical properties of SLs one should know the complete information on their crystal structure. When analysing the SL structure, we first adopt an approximation that the atoms in SLs are on the sites of a zinc-blende lattice with lattice constant a being an average

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of the two lattice parameters of GaAs and AlAs. This can be done since the difference in the lattice constants of GaAs and AlAs is less than 0.2%. Taking this approximation into account the coordinates of all the atoms in the lattice are well defined. So one can determine both the space group and the atomic arrangement over the Wyckoff positions for a SL with arbitrary numbers of monolayers m and n .

For the [001] orientation of layers, the space groups have been determined in [6] and the distribution of atoms in the primitive cell have been obtained in our previous papers [1, 2]. For other orientations the structure information is not sufficient. The space groups only have been found for the [110] [7] and [111] [8] growth directions whereas the arrangement of atoms over the Wyckoff positions in a primitive cell has not been analysed. No result, according to our knowledge, has been published concerning the symmetry properties of the electron states in SLs grown in the [110] and [111] directions.

The SLs can be considered as new crystals with an enlarged unit cell compared with that of parent materials (GaAs and AlAs in our case). Nevertheless, the SL electron states appear to ‘remember’ their genesis, i.e. from which band states of parent materials they have arisen. Therefore, it is worth performing some preliminary symmetry analysis of SLs based on the properties of bulk materials.

GaAs and AlAs single crystals have the zinc-blende structure (space group T_d^2) with very close lattice parameters. In both crystals, the top of the valence band is located at the Γ point in the Brillouin zone (BZ) of the fcc lattice whereas the bottom of the conduction band is located respectively at the Γ point for GaAs and at the X point for AlAs. The energy in the conduction band at the L point is intermediate between those of the X and Γ points in both crystals [9].

For the $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs, in the reduced-zone approximation, the folding of the bulk material BZ over the superlattice BZ (SLBZ) along the z -axis (growth direction) puts the X_z point of the bulk material in correspondence with a point either at the centre or at the surface of the SLBZ depending on whether $m+n$ is even or odd. (The X_x and X_y points of the bulk BZ are always related to points at the SLBZ surface.) It is generally admitted that the top of the valence band is located at the Γ point of the SLBZ whereas the position of the bottom of the conduction band in the SLBZ depends on the thicknesses of the GaAs and AlAs slabs. This leads to two types of SL.

(i) If the eigenstate with the minimal energy in the conduction band originates from the Γ point in the GaAs BZ, it is located at the Γ point of the SLBZ; the electrons and holes are then localized in GaAs regions and the SL is type I.

(ii) If the eigenstate with the minimal energy originates from the X_z point in the AlAs BZ, it is located at the Γ point of the SLBZ if $m+n$ is even and at a point on the surface of the SLBZ if $m+n$ is odd. In both cases electrons are localized in AlAs regions, i.e. the electrons and holes are spatially separated; in the former case the optical transition is direct in k -space and indirect in real space and the SL is pseudodirect type II (moreover, it has been claimed that the parity of the wavefunction in the conduction band under the change of z into $-z$ is that of n [10]); in the latter case the transition is indirect in both k - and real space and the SL is type II. Last, if the eigenstate with the minimal energy originates from the X_{xy} point in the AlAs BZ, it is located on the surface of the SLBZ and the electrons are localized in AlAs regions; the transition is indirect in both k - and real space and the SL is type II.

Note that, for direct type I SLs, there are allowed optical transitions at the Γ point. When Γ - Γ transitions are allowed from symmetry in the pseudodirect SLs, they should have a weak intensity since the overlap of electron and hole envelope functions is small.

The type (I or II) of $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs has been extensively studied by different optical techniques: absorption [11], optically detected magnetic resonance [12], photoluminescence under hydrostatic pressure [9], etc. For SLs with $m = n$, the estimated values of m at which the type I to type II transition takes place present discrepancies from one author to another; often it is even claimed that the transition occurs between $m = 10$ and $m = 14$. On the other hand, the electron-band structures of GaAs/AlAs short-period SLs have been calculated using various methods. Most of the results converge to the $m = 8$ – 13 interval for the type I to type II transition to occur when $n = m$ [9].

In this paper, we analyse the electron state symmetries at the symmetry points of the BZ for the $(\text{GaAs})_m(\text{AlAs})_n$ SLs grown along the [001] direction. Next, we derive the selection rules for optical transitions in these materials. Finally, based on our group-theory results and electronic-structure calculations made by other authors, we predict which lines could be expected to be observed in polarized optical spectra. The results concerning the dependence of a crystal structure on the numbers of monolayers m and n for the $(\text{GaAs})_m(\text{AlAs})_n$ SLs grown along the [110] and [111] directions as well as the symmetry analysis of electron states and optical selection rules will be published in a separate paper.

2. Electron state symmetry

The crystal structures of typical representatives of the two different families of $(\text{GaAs})_m(\text{AlAs})_n$ SLs grown along the [001] direction are presented in figures 1 and 2. The two families correspond to even and odd values of $m + n$. The figures also show the BZs for the corresponding space groups, D_{2d}^5 and D_{2d}^9 . The formulae giving the atomic arrangements over the Wyckoff positions are presented in table 1 (see also [1] and [2]). Here, the numbers preceding the chemical element symbols denote the number of such atoms at the Wyckoff positions shown in parentheses. Analysing table 1 one can see that each of the crystal families can be subdivided into several subfamilies specified by non-equivalent types of atomic arrangement over the Wyckoff positions.

Table 1. Atomic arrangements over the Wyckoff positions in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs

Space group D_{2d}^5 ($P\bar{4}m2$), $m + n = 2k$, $m \leq n$					
$m = 2k + 1$, $n = 2s + 1$				$m = 2k$, $n = 2s$	
$m = 4i + 1$	$m = 4i + 3$	$m = 4i + 1$	$m = 4i + 3$	$m + n = 4i$	$m + n = 4i + 2$
$n = 4j + 3$	$n = 4j + 1$	$n = 4j + 1$	$n = 4j + 3$		
1Ga(1a)				mGa(2g)	
$(m + n)\text{As}(2g)$				nAl(2g)	
1Al(1d)		1Al(1c)		1As(1a)	
$\frac{m-1}{2}\text{Ga}(2f)$	$\frac{m+1}{2}\text{Ga}(2f)$	$\frac{m-1}{2}\text{Ga}(2f)$	$\frac{m+1}{2}\text{Ga}(2f)$	1As(1d)	1As(1c)
$\frac{m-1}{2}\text{Ga}(2e)$	$\frac{m-3}{2}\text{Ga}(2e)$	$\frac{m-1}{2}\text{Ga}(2e)$	$\frac{m-3}{2}\text{Ga}(2e)$	$\frac{m+n}{2}\text{As}(2f)$	$(\frac{m+n}{2} - 1)\text{As}(2f)$
$\frac{n+1}{2}\text{Al}(2f)$	$\frac{n-1}{2}\text{Al}(2f)$	$\frac{n-1}{2}\text{Al}(2f)$	$\frac{n-3}{2}\text{Al}(2f)$	$(\frac{m+n}{2} - 2)\text{As}(2e)$	$(\frac{m+n}{2} - 1)\text{As}(2e)$
$\frac{n-3}{2}\text{Al}(2e)$	$\frac{n-1}{2}\text{Al}(2e)$	$\frac{n-1}{2}\text{Al}(2e)$	$\frac{n+1}{2}\text{Al}(2e)$		
Space group D_{2d}^9 ($I\bar{4}m2$), $m + n = 2k + 1$					
$m = 2k + 1$, $n = 2s$			$m = 2k$, $n = 2s + 1$		
1Ga(1a) 1As(1c) nAl(2e)			1As(1a) 1Al(1c) mGa(2f)		
$(m - 1)\text{Ga}(2e)$ $(m + n - 1)\text{As}(2f)$			$(n - 1)\text{Al}(2f)$ $(m + n - 1)\text{As}(2e)$		

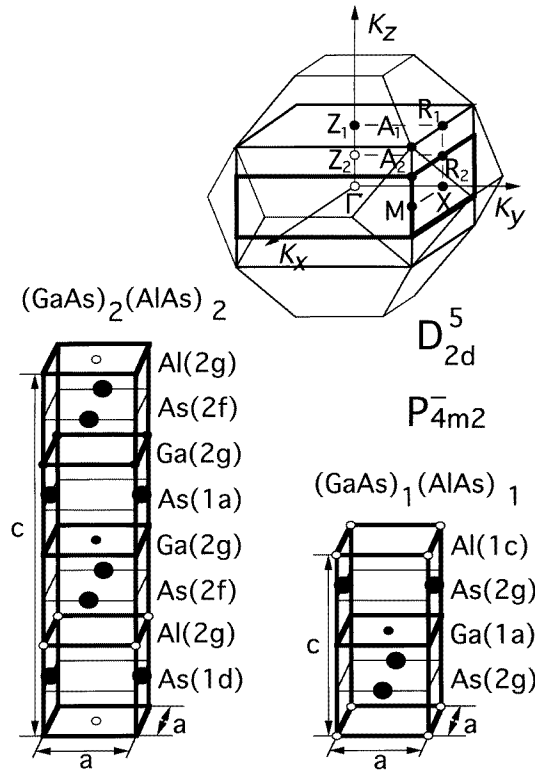


Figure 1. The crystal structures and corresponding BZs of $(\text{GaAs})_2(\text{AlAs})_2$ and $(\text{GaAs})_1(\text{AlAs})_1$ [001]-grown superlattices.

For the D_{2d}^5 crystal family, there are four SL subfamilies corresponding to odd numbers of both GaAs and AlAs monolayers and two SL subfamilies with even m and n . For the four former subfamilies, high-symmetry sites (D_{2d} —1a, 1c, and 1d) in the lattice are occupied by metal (Me = Ga, Al) atoms, whereas all As atoms are in low-symmetry Wyckoff positions (C_{2v} —2e, 2f, and 2g). The difference between the four subfamilies is subtle and results in the variations of occupation numbers of Wyckoff positions with the same site symmetry by atoms of the same type. Thus, the period of atomic arrangements over the Wyckoff positions is equal to four for both m and n . For the two latter subfamilies, the Me and As atoms interchange their sites, that is, high-symmetry positions are occupied by As atoms, whereas all the metal atoms arrange at low-symmetry sites. In this case, the period of atomic arrangements over the Wyckoff positions is equal to four for $m + n$.

For the D_{2d}^9 crystal family, there are two subfamilies of SLs corresponding to either odd numbers of GaAs and even numbers of AlAs monolayers or *vice versa*. When m is odd and n is even, there is no Al atom in a D_{2d} -symmetry position, whereas none of Ga atoms is placed at a D_{2d} -symmetry site when m and n change the parities.

Knowing the space groups and atomic arrangements, one can determine the symmetry of electron states in the $(\text{GaAs})_m(\text{AlAs})_n$ SLs using the method of induced band representations of space groups. The main concepts of this method are given elsewhere [2, 13–16]. It allows one to establish a symmetry correspondence between extended (Bloch) and localized (Wannier-type) one-electron states in crystals. The electron state symmetries for different

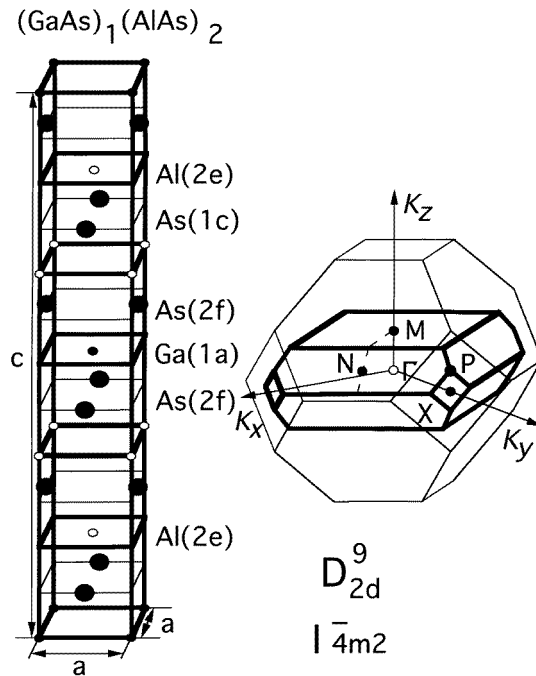


Figure 2. The crystal structure and corresponding BZ of a $(\text{GaAs})_1(\text{AlAs})_2$ [001]-grown superlattice.

SLs are presented in tables 2 and 3. These tables have the following structure. Columns 1–6 contain the atomic arrangements over the Wyckoff positions (sites in direct space) given in column 7 together with their coordinates (in units of translation vectors of the crystallographic unit cell) and site symmetry groups. Column 8 contains the Mulliken symbols of those irreducible representations (irreps) of the site symmetry groups for these Wyckoff positions, according to which the localized one-electron wave functions transform, as well as the symbols of double-valued irreps (denoted by a bar over the irrep symbol) in the case where the spin–orbit interaction is taken into account.

We do not specify the explicit form of the localized functions. Their spatial distributions within the primitive cell remain undefined in terms of the group theory. In the symmetry analysis, only transformation properties of these functions are important, being described by the irreps of the site symmetry group of corresponding atoms. It should be noted that though the Wannier-type orbitals may differ from the corresponding atomic orbitals (s , p , d , etc) they transform according to the same irreps of a site symmetry group.

The remaining columns of tables 2 and 3 give the labels of single- and double-valued induced representations in the k -basis, with the symbols of k -points (wave vectors), their coordinates (in units of primitive translations of the reciprocal lattice), and their point groups in rows 1–3 respectively, and the indices of small irreps of little groups in subsequent rows; these determine the symmetries of electron band states (Bloch states). In these tables and in each of the following ones, the labelling of the space groups irreps is that of [17], the labelling of the point-group irreps is that of [18], and the site points q are indexed as Wyckoff positions from [19].

Table 2. Electron state symmetries in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group $D_{2d}^5(P\bar{4}m2)$.

$m = 1$ $n = 1$	$m = 2$ $n = 2$	$m = 1$ $n = 3$	$m = 1$ $n = 5$	$m = 2$ $n = 4$	$m = 3$ $n = 3$	D_{2d}^5 $(P\bar{4}m2)$	Γ (000) D_{2d}	M $(\frac{1}{2}\frac{1}{2}0)$ D_{2d}	A $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ D_{2d}	Z $(00\frac{1}{2})$ D_{2d}	X $(0\frac{1}{2}0)$ C_{2v}	R $(0\frac{1}{2}\frac{1}{2})$ C_{2v}
1Ga	1As	1Ga	1Ga	1As	1Ga	$a_1(s)$	1	1	1	1	1	1
						$b_2(p_z)$	2	2	2	2	1	1
						1a (000) $e(p_x, p_y)$	5	5	5	5	3,4	3,4
						\bar{e}_1	6	6	6	6	5	5
						D_{2d} \bar{e}_2	7	7	7	7	5	5
1Al	—	—	1Al	1As	1Al	$a_1(s)$	1	4	3	2	3	3
						$b_2(p_z)$	2	3	4	1	3	3
						1c $e(p_x, p_y)$	5	5	5	5	1,2	1,2
						$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ \bar{e}_1	6	7	6	7	5	5
						D_{2d} \bar{e}_2	7	6	7	6	5	5
—	1As	1Al	—	—	—	$a_1(s)$	1	1	2	2	1	1
						$b_2(p_z)$	2	2	1	1	1	1
						1d $e(p_x, p_y)$	5	5	5	5	3,4	3,4
						$(00\frac{1}{2})$ \bar{e}_1	6	6	7	7	5	5
						D_{2d} \bar{e}_2	7	7	6	6	5	5
—	—	—	2Al	2As	2Al	$a_1(s; p_z)$	1,2	1,2	1,2	1,2	1,1	1,1
						2e $b_2(p_y)$	5	5	5	5	3,4	3,4
						(00z) $b_1(p_x)$	5	5	5	5	3,4	3,4
						C_{2v} \bar{e}	6,7	6,7	6,7	6,7	5,5	5,5
—	2As	2Al	2Al	2As	2Ga	$a_1(s; p_z)$	1,2	3,4	3,4	1,2	3,3	3,3
						2f $b_2(p_y)$	5	5	5	5	1,2	1,2
						$(\frac{1}{2}\frac{1}{2}z)$ $b_1(p_x)$	5	5	5	5	1,2	1,2
						C_{2v} \bar{e}	6,7	6,7	6,7	6,7	5,5	5,5
2As	2Al	4As	6As	4Al	6As	$a_1(s; p_z)$	1,2	5	5	1,2	1,3	1,3
	2Ga			2Ga		2g $b_2(p_y)$	5	1,2	1,2	5	1,4	1,4
						$(0\frac{1}{2}z)$ $b_1(p_x)$	5	3,4	3,4	5	2,3	2,3
						C_{2v} \bar{e}	6,7	6,7	6,7	6,7	5,5	5,5

We limit ourselves to the s and p atomic-like localized states (one s state and three p states per atom) since just these functions form the uppermost valence-band states and the lowest conduction-band states and, therefore, determine the interband optical transitions. Nevertheless, to describe the lower valence-band states and upper conduction-band ones, the d states should be also taken into consideration. This could be done using a similar procedure.

From tables 2 and 3 one can easily write down the symmetry of the electron states at symmetry points of the SLBZ and determine which localized states and which atoms in a primitive cell contribute to them.

For example, in the $(\text{GaAs})_1(\text{AlAs})_1$ SL (in a short notation, the (1×1) SL), the s-atomic-like Wannier-type orbital corresponding to the Al atom in the 1c Wyckoff position (for short, the s orbital of Al) induces non-degenerate Bloch states Γ_1 , M_4 , A_3 , Z_2 , X_3 , and R_3 (see table 2). Thus, 1 in the column Γ means small irrep Γ_1 , 4 in the column M means M_4 , etc. We can also see that Γ_1 states are induced by s orbitals of Ga and Al as well as by s and p_z orbitals of As, Γ_2 states are formed by p_z orbitals of Ga and Al and by s and p_z orbitals of As, and, finally Γ_5 states are formed by p_x and p_y orbitals of Ga, Al, and As atoms. Thus, at the Γ point we have four Γ_1 , four Γ_2 , and four Γ_5 Bloch states resulting

Table 3. Electron state symmetries in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group $D_{2d}^9(I\bar{4}m2)$ (co-rep: $N_3 + N_4$).

$m = 1$ $n = 2$	$m = 2$ $n = 3$	$m = 1$ $n = 4$	$m = 1$ $n = 6$	$m = 2$ $n = 5$	$m = 3$ $n = 6$	D_{2d}^9 ($I\bar{4}m2$)	Γ (000) D_{2d}	M $(\frac{1}{2}\frac{1}{2} - \frac{1}{2})$ D_{2d}	X $(00\frac{1}{2})$ D_2	P $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ S_4	N $(0\frac{1}{2}0)$ C_s
1Ga	1As	1Ga	1Ga	1As	1Ga	$a_1(s)$	1	1	1	1	1
						$b_2(p_z)$	2	2	2	2	1
						1a $e(p_x, p_y)$	5	5	3,4	3,4	1,2
						(000) \bar{e}_1	6	6	5	5,7	3,4
						D_{2d} \bar{e}_2	7	7	5	6,8	3,4
1Al	1Al	1As	1As	1Al	1As	$a_1(s)$	1	2	3	4	1
						$b_2(p_z)$	2	1	4	3	1
						1c $e(p_x, p_y)$	5	5	1,2	1,2	1,2
						$(0\frac{1}{2}\frac{1}{4})$ \bar{e}_1	6	7	5	6,7	3,4
						D_{2d} \bar{e}_2	7	6	5	5,8	3,4
2Al	4As	4Al	6Al	6As	4Al	$a_1(s; p_z)$	1,2	1,2	1,2	1,2	1,1
					2Ga	2e $b_2(p_y)$	5	5	3,4	3,4	1,2
						(00 $_z$) $b_1(p_x)$	5	5	3,4	3,4	1,2
						C_{2v} \bar{e}	6,7	6,7	5,5	5,6,7,8	3,3,4,4
2As	2Al	4As	6As	4Al	6As	$a_1(s; p_z)$	1,2	1,2	3,4	3,4	1,1
	2Ga				2Ga	2f $b_2(p_y)$	5	5	1,2	1,2	1,2
						$(0\frac{1}{2}z)$ $b_1(p_x)$	5	5	1,2	1,2	1,2
						C_{2v} \bar{e}	6,7	6,7	5,5	5,6,7,8	3,3,4,4

from s and p localized states (Ga, Al, and As atoms). We can conclude, for example, that the Bloch states induced by p_x and p_y orbitals of Ga, Al, and As atoms do not mix at the Γ point with the states induced by s and p_z orbitals since they have different symmetries. These results could significantly simplify the numerical calculations of electron-band structures of these materials since for each particular band state we could limit the number of Wannier-type orbitals that should be taken into account. This is especially important if the number of atoms per primitive cell is very large, and that is the case for most SLs. For example, for the (1×1) SL one can see that only s orbitals of Al and p_x orbitals of As contribute to the states M_4 . Our group-theory results agree with the numerical calculations of contributions of different orbitals to SL band states made in [20] (see table IV therein). For example, for the M_4 state with energy of 3.14 eV the following relative contributions of different atomic orbitals (i.e. the percentages of s and p states within the atomic spheres for each type of atom) were obtained in [20]: Ga, s—0, p—0; Al, s—19.9, p—0; As, s—0, p—7.3. This agrees with the symmetry-analysis results given in table 2. Note that the authors of [20] do not distinguish the contributions of different p states as we do.

Analysing the results given in tables 2 and 3, one can formulate in terms of site symmetry the definition of type-I and type-II SLs. The difference between these two types is the following: in the type-I SLs, the crystalline orbitals corresponding to the top of the valence band and to the bottom of the conduction band should include orbitals of atoms belonging to the layers of the same type (GaAs or AlAs). In the type-II SLs, these crystalline orbitals should not. In the present description, the As atoms lying at the interfaces have obviously to be considered as belonging to both types of layer. The site-symmetry method therefore allows one to establish qualitatively localizations of different crystalline orbitals.

Below, we speak about localization in the sense that the atoms from layers of only one type (GaAs or AlAs) contribute to a particular crystalline state. For example, for the (1×1)

SL (see table 2), the Bloch states Γ_1 , M_1 , A_1 , Z_1 , X_1 , and R_1 induced by s orbitals of Ga atoms are periodically localized in GaAs regions whereas the Bloch states Γ_1 , M_4 , A_3 , Z_2 , X_3 , and R_3 induced by s orbitals of Al atoms are periodically localized in AlAs regions. For the (2×2) SL, Bloch states Γ_1 , M_1 , A_1 , Z_1 , X_1 , and R_1 , which are induced by As atoms lying between Ga planes, are also periodically localized in the GaAs regions though having another energy. Besides, the s and p_z states of Ga and Al atoms contribute to the composite Bloch states with the same symmetries (Γ_1 , Γ_2), M_5 , A_5 , (Z_1, Z_2), (X_1, X_3), and (R_1, R_3).

In many papers the problem of Γ - X mixing is studied both theoretically and experimentally (for references, see e.g. [9], [10] and [21]). When there is no external perturbation, two states Ψ_i and Ψ_j mix if they have the same energy and if their overlap integral is not equal to zero: $\langle \Psi_i | \Psi_j \rangle \neq 0$. There is therefore no mixing if the symmetries of states Ψ_i and Ψ_j are different.

In the reduced-zone approximation, one uses bulk wave functions in both GaAs and AlAs slabs. In the case of the Γ - X_z mixing, the conduction-band wave function has the Γ symmetry in the GaAs slabs and the X_z symmetry in the AlAs ones. When both parts of the wave function correspond to the same energy (the confinement energy being included), the SL potential introduced with interface discontinuities lifts this degeneracy if it is allowed from parity. The perturbed wave functions are then linear combinations of the former Γ and X_z wave functions and no longer have any defined symmetry [22]. In our site-symmetry analysis, the exact symmetries of the wave functions are provided, and only a further perturbation potential could mix the exact eigenfunctions. Such a potential could arise, for example, from impurities, defects, applied fields, strains, etc.

Finally, if we take the spin-orbit interaction into consideration, the s, p, etc orbitals are replaced by the $|J, m_J\rangle$ orbitals where J and m_J are the total angular momentum and its projection. The corresponding double-valued induced representations are given in tables 2 and 3. For example, for the (1×1) SL, the s-derived $|\frac{1}{2}, \pm\frac{1}{2}\rangle$ and p-derived $|\frac{3}{2}, \pm\frac{3}{2}\rangle$ states localized at the Ga positions transform according to double-valued irrep \bar{e}_1 whereas p-derived ones $|\frac{3}{2}, \pm\frac{1}{2}\rangle$ and $|\frac{1}{2}, \pm\frac{1}{2}\rangle$ transform according to \bar{e}_2 . As a result, the $4\Gamma_1 + 4\Gamma_2 + 4\Gamma_5$ states will become the $8\Gamma_6 + 8\Gamma_7$ ones.

3. Optical transition selection rules

The selection rules for optical transitions follow from the symmetry restrictions imposed on matrix elements of transitions from an initial (i) electron state to a final (f) one under the action of the perturbative operator W . In terms of group theory, for a system having the space group G , the optical transition matrix elements do not vanish due to symmetry if the following Kronecker products of reps of G contain the identity irrep

$$(D^f)^* \times D^W \times D^i \supset \Gamma_1. \quad (1)$$

Here D^i and D^f are the irreps of the space group G according to which the initial and final electron states are transformed, D^W is the rep according to which the perturbative operator W is transformed and Γ_1 is the identity irrep of the group G .

In light absorption processes, the perturbative operator is $W \propto (\mathbf{e} \cdot \mathbf{p}) \exp(i\mathbf{k} \cdot \mathbf{r})$, where \mathbf{e} and \mathbf{k} are the polarization and wave vector of light, respectively, and \mathbf{p} is the momentum operator of an electron. For the light frequency range the condition $k_i a \ll 1$ (where a is the lattice parameter) is satisfied; that leads to an approximation called the dipole approximation:

$$W \propto (\mathbf{e} \cdot \mathbf{p}). \quad (2)$$

Thus, the perturbative operator W transforms according to the vector representation D^v of the space group G . Hence, the transitions are allowed between those pairs of electron states D^f and D^i which obey the condition

$$(D^f)^* \times D^i \cap D^v \neq 0. \quad (3)$$

Since the reps according to which the perturbative operator W is transformed correspond to the zero wave vector, only those combinations of electron states for which the Kronecker product contains the rep with $\mathbf{k} = \mathbf{0}$ can be allowed.

In tables 4 and 5, for the space groups D_{2d}^5 and D_{2d}^9 respectively, we present the $\mathbf{k} = \mathbf{0}$ parts of Kronecker products of irreps corresponding to various combinations of initial and final electron states at the symmetry points of SLBZ. For example, $X_1 \times X_4 = \Gamma_5 + M_5$, and + in the column Γ_5 means that this irrep forms part of the direct product. The transitions are allowed between those pairs of states for which Kronecker products have irreps in common with the vector representation. For the space groups D_{2d}^5 and D_{2d}^9 , the vector representation is $D^v = \Gamma_2(z) + \Gamma_5(x, y)$. Thus, the optical transition between the states X_1 and X_4 —taken above as an example—is allowed in the x and y polarizations and forbidden in the z polarization.

Table 4. Selection rules for direct optical transitions in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group D_{2d}^5 .

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Allowed polarizations
Single-valued irreps						
$D = \Gamma, M, A, Z$						
$D_i \times D_i$ ($i = 1-4$)	+					forbidden
$D_1 \times D_2, D_3 \times D_4$		+				z
$D_1 \times D_3, D_2 \times D_4$			+			forbidden
$D_1 \times D_4, D_2 \times D_3$				+		forbidden
$D_i \times D_5$ ($i = 1-4$)					+	x, y
$D_5 \times D_5$	+	+	+	+		z
$D = X, R$						
$D_i \times D_i$ ($i = 1-4$)	+	+				z
$D_1 \times D_2, D_3 \times D_4$			+	+		forbidden
$D_i \times D_j$ ($i = 1, 2; j = 3, 4$)					+	x, y
Double-valued irreps (with spin-orbit interaction included)						
$D = \Gamma, M, A, Z$						
$D_i \times D_i$ ($i = 6, 7$)	+		+		+	x, y
$D_6 \times D_7$		+		+	+	$x, y; z$
$D = X, R$						
$D_5 \times D_5$	+	+	+	+	+	$x, y; z$

When the spin-orbit interaction is taken into account, the products of double-valued irreps should be considered. The symmetry correspondence between the Bloch states which transform according to single-valued irreps (without spin-orbit coupling) and those which transform according to the double-valued irreps (with spin-orbit coupling) can be obtained as follows. The Bloch state D^l ($l = s, p$) corresponds to the states which transform according to the double-valued representation $\bar{D}^J = D^l \times \bar{D}^{1/2}$ where $\bar{D}^{1/2}$ is the double-valued irrep according to which the spinor function is transformed. For the space groups D_{2d}^5 and D_{2d}^9 , the spinor function is transformed according to $\bar{D}^{1/2} = \bar{e}_1$. Decomposing the corresponding direct products of coordinate and spinor parts of the one-electron wave function, we obtain

Table 5. Selection rules for direct optical transitions in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group D_{2d}^9 .

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Allowed polarizations
Single-valued irreps						
$D = \Gamma, M$						
$D_i \times D_j$ ($i = 1-4$)	+					forbidden
$D_1 \times D_2, D_3 \times D_4$		+				z
$D_1 \times D_3, D_2 \times D_4$			+			forbidden
$D_1 \times D_4, D_2 \times D_3$				+		forbidden
$D_1 \times D_5$ ($i = 1-4$)					+	x, y
$D_5 \times D_5$	+	+	+	+		z
$X_i \times X_j$ ($i = 1-4$)	+			+		forbidden
$X_1 \times X_2, X_3 \times X_4$		+	+			z
$X_i \times X_j$ ($i = 1, 2; j = 3, 4$)					+	x, y
$P_1 \times P_1, P_2 \times P_2$	+			+		forbidden
$P_3 \times P_3, P_4 \times P_4$	+		+			forbidden
$P_1 \times P_2, P_3 \times P_4$		+		+		z
$P_i \times P_j$ ($i = 1, 2; j = 3, 4$)					+	x, y
$N_i \times N_j$ ($i = 1, 2$)	+	+			+	$x, y; z$
$N_1 \times N_2$			+	+	+	x, y
Double-valued irreps (with spin-orbit interaction included)						
$\Gamma_i \times \Gamma_i$ ($i = 6, 7$)	+		+		+	x, y
$\Gamma_6 \times \Gamma_7$		+		+	+	$x, y; z$
$M_i \times M_i$ ($i = 6, 7$)	+		+		+	x, y
$M_6 \times M_7$		+		+	+	$x, y; z$
$X_5 \times X_5$	+	+	+	+	+	$x, y; z$
$P_i \times P_i$ ($i = 5-8$)	+		+			forbidden
$P_5 \times P_6, P_7 \times P_8$		+		+		z
$P_i \times P_j$ ($i = 5, 6; j = 7, 8$)					+	x, y
$N_i \times N_i$ ($i = 3, 4$)			+	+	+	x, y
$N_3 \times N_4$	+	+			+	$x, y; z$

the set of states into which D^l transforms when the spin-orbit interaction is included. At the Γ point of the BZ, the symmetry correspondence is $\Gamma_1 \rightarrow \Gamma_6, \Gamma_2 \rightarrow \Gamma_7, \Gamma_5 \rightarrow \Gamma_6 + \Gamma_7$, and at the M point $M_1 \rightarrow M_6, M_2 \rightarrow M_7, M_3 \rightarrow M_6, M_4 \rightarrow M_7, M_5 \rightarrow M_6 + M_7$.

As a result, we obtain a relation between the selection rules when the spin-orbit interaction is taken into account (lower parts of tables 4 and 5) and those when it is not (upper parts). It can be seen that some forbidden transitions become allowed when the spin-orbit interaction is taken into account (table 6).

Besides direct optical transitions, the phonon-assisted ones may be of importance. The phonon-assisted optical transitions are allowed between those initial and final electron states belonging to different points of the BZ which obey the following conditions:

$$(D^{virt})^* \times D^i \cap D^v \neq 0 \quad (D^{virt})^* \times D^{ph} \times D^f \supset \Gamma_1 \quad (4a)$$

where D^{virt} and D^{ph} are the irreps according to which the virtual electron and phonon state are transformed. In the case (4a), the virtual electron state belongs to the same wave vector as an initial state. Other transitions are also possible, with the virtual electron state belonging to the same wave vector as a final state. In the latter case, the states obey the

Table 6. The modification of selection rules for direct optical transitions when including spin-orbit interaction (space groups D_{2d}^5 and D_{2d}^9). The labels of both the irreps and additional light polarizations (x , y , or z) in parentheses refer to the case where spin-orbit coupling is taken into account.

		Conduction-band states			
		$\Gamma_1(\Gamma_6)$	$\Gamma_2(\Gamma_7)$	$\Gamma_5(\Gamma_6)$	$\Gamma_5(\Gamma_7)$
Valence-band states	$\Gamma_1(\Gamma_6)$	(x, y)	$(x, y)z$	x, y	$x, y(z)$
	$\Gamma_2(\Gamma_7)$	$(x, y)z$	(x, y)	$x, y(z)$	x, y
	$\Gamma_5(\Gamma_6)$	x, y	$x, y(z)$	(x, y)	$(x, y)z$
	$\Gamma_5(\Gamma_7)$	$x, y(z)$	x, y	$(x, y)z$	(x, y)

following conditions:

$$(D^i)^* \times D^{ph} \times D^{virt} \supset \Gamma_1 \quad (D^f)^* \times D^{virt} \cap D^v \neq 0. \quad (4b)$$

For the short-period SLs under consideration, there is a consensus among all the published calculations that the uppermost valence-band states at the Γ point are about 1 eV higher in energy than the states at the other symmetry points [20, 23–27]. Therefore, due to such a large difference in energy, one can neglect the transitions via the virtual valence-band states at symmetry points with $\mathbf{k} \neq \mathbf{0}$. By doing this, one has to consider only the (4a) transitions for the optical absorption spectra and the (4b) ones for the luminescence spectra. Transitions involving optical phonons with $\mathbf{k} = \mathbf{0}$ (the Γ_1 , Γ_2 , and Γ_5 optical phonons) are also to be considered in the case where two conduction bands and/or two valence bands have energies close to one other at the Γ point.

Using tables 4 and 5, one can obtain the selection rules for phonon-assisted optical transitions. Such rules for the D_{2d}^5 and D_{2d}^9 space groups are presented in tables 7 and 8. If one takes into consideration the spin-orbit interaction, the rules are modified (tables 9 and 10 for the D_{2d}^5 and D_{2d}^9 space groups, respectively). In addition, in tables 9 and 10 those transitions involving the optical Γ phonons are included, which obey the (4b) conditions. Note that one can practically always find appropriate phonons for the indirect transitions. These transitions are allowed between those initial and virtual states (in case (4a)) or virtual and final ones (in case (4b)) for which Kronecker products have irreps in common with the vector representation, that is to say, for which the zero-phonon transitions are allowed.

Thus, a particular interband transition can be allowed either completely or in certain polarizations due to the appropriate symmetries of involved states, and/or due to the spin-orbit interaction, and/or due to the electron-phonon interaction. In the two latter cases, its oscillator strength will be weak. It is worth noting that the oscillator strength is also determined by atomic arrangement in the Wyckoff positions. The higher the occupation number of a position, the greater the strength of a transition involving band states induced by the atoms in this position. This can be considered in terms of the ‘bulk genesis’ of some bands when the number of GaAs and/or AlAs layers is rather high, that is to say when the occupation numbers of some Wyckoff positions are much larger than those of others (by an order of magnitude or more).

Of course, the most important ones are the transitions between the uppermost states in the valence band and the lowest states in the conduction band. Group-theory analysis alone does not permit us to determine even the relative energy positions of different states. It is possible only to assume that relative energy positions of different band states could change when m and n are varied. This is due to the fact that distinct localized functions contribute to the band states with the same symmetry in different SLs. For example, one

Table 7. Selection rules for phonon-assisted optical transitions in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group D_{2d}^5 (neglecting the spin-orbit interaction).

Initial state (valence band)	Virtual state (conduction band)	Final state (conduction band)	Assisting phonons ^a	Allowed polarizations	
Γ_1	Γ_1	any	any	forbidden	
		Γ_2	D_i	D_j $D = \Gamma, M, A, Z$ $(i, j) = (1, 2); (2, 1); (3, 4); (4, 3); (5, 5)$	z
	D_i		D_i $D = R, X$		
	Γ_5	D_5	$D_1 + D_2 + D_3 + D_4$	x, y	
		D_i ($i \neq 5$)	D_5 $D = \Gamma, M, A, Z$		
		D_i ($i = 1, 2$)	$D_3 + D_4$		
D_i ($i = 3, 4$)		$D_1 + D_2$ $D = X, R$			
Γ_2	Γ_1	D_i	D_i $D = \Gamma, M, R, X, A, Z$	z	
		Γ_2	any	any	forbidden
	Γ_5		D_5	$D_1 + D_2 + D_3 + D_4$	x, y
			D_i ($i \neq 5$)	D_5 $D = \Gamma, M, A, Z$	
			D_i ($i = 1, 2$)	$D_3 + D_4$	
		D_i ($i = 3, 4$)	$D_1 + D_2$ $D = X, R$		
Γ_5	Γ_1	D_i	D_i $D = \Gamma, M, R, X, A, Z$	x, y	
		Γ_2	D_i	D_j $D = \Gamma, M, A, Z$ $(i, j) = (1, 2); (2, 1); (3, 4); (4, 3); (5, 5)$	x, y
	D_i		D_i $D = R, X$		
	Γ_5		D_5	$D_1 + D_2 + D_3 + D_4$	z
			D_i ($i \neq 5$)	D_5 $D = \Gamma, M, A, Z$	
		D_i ($i = 1, 2$)	$D_3 + D_4$		
		D_i ($i = 3, 4$)	$D_1 + D_2$ $D = X, R$		

^a The Γ_3 , Γ_4 , Z_3 and Z_4 phonons are absent (see e.g. [2]).

can see for the (2×2) and (1×3) SLs that As and Me (Ga and Al) atoms interchange their positions, i.e. in the (2×2) SL the a, d, and f Wyckoff positions are occupied by As atoms and g positions by Ga and Al atoms whereas in the (1×1) SL the As atoms replace Me atoms and, in turn, Me atoms replace As. It is clear that the number of band states with a particular symmetry depends completely on which Wyckoff positions are occupied and which not whereas the energies of these states depend on the chemical nature of elements that occupy these positions. Such rearrangement of atoms over the Wyckoff positions as for (1×1) and (2×2) SLs will ultimately result in relative shifts of band states on the energy scale. This is a qualitative picture of this effect. However, some predictions could be made only by comparison with the band-structure calculations [20, 23–27] (see below).

4. Discussion

There are many contradictions in the results of electronic-structure calculations given by different authors [20, 23–27]. Therefore, it is worth giving a comparative analysis of different methods presently used because several review papers devoted to this problem

Table 8. Selection rules for phonon-assisted optical transitions in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group D_{2d}^9 (neglecting the spin-orbit interaction).

Initial state (valence band)	Virtual state (conduction band)	Final state (conduction band)	Assisting phonons	Allowed polarizations
Γ_i ($i = 1, 2$)	Γ_i ($i = 1, 2$)	any	any	forbidden
Γ_1	Γ_2	D_i L_i N_i ($i = 1, 2$)	D_j L_j N_j $(i, j) = (1, 2); (2, 1); (5, 5)$ $(i, j) = (1, 2); (2, 1); (3, 4); (4, 3)$	$D = \Gamma, M$ $L = X, P$ z
Γ_2	Γ_1	D_i	D_i	$D = \Gamma, M^a, X, P, N$ z
Γ_i ($i = 1, 2$)	Γ_5	D_5 D_i ($i = 1, 2$) L_i ($i = 1, 2$) L_j ($i = 3, 4$) N_i ($i = 1, 2$)	$D_1 + D_2$ D_5 $L_3 + L_4$ $L_1 + L_2$ $N_1 + N_2$	$D = \Gamma, M$ $L = X, P$ x, y
Γ_5	Γ_1	D_i	D_i	$D = \Gamma, M^a, X, P, N$ x, y
	Γ_2	D_i L_i N_i ($i = 1, 2$)	D_j L_j N_j $(i, j) = (1, 2); (2, 1); (5, 5)$ $(i, j) = (1, 2); (2, 1); (3, 4); (4, 3)$	$D = \Gamma, M$ $L = X, P$ x, y
	Γ_5	D_5 D_i ($i = 1, 2$) L_i ($i = 1, 2$) L_j ($i = 3, 4$) N_i ($i = 1, 2$)	$D_1 + D_2$ D_5 $L_3 + L_4$ $L_1 + L_2$ $N_1 + N_2$	$D = \Gamma, M$ $L = X, P$ z

^a The $\Gamma_3, \Gamma_4, M_3,$ and M_4 phonons are absent (see e.g. [2]).

(see, e.g., [10], [21] and [28]) did not treat short-period SLs in a completely satisfactory way.

We may divide all the approaches used into the ones based on the properties of constituent compounds and those dealing with the SL as a new crystal.

(i) The approaches of the first type are called ‘engineering methods’ [21] or ‘boundary-condition approaches’ [28]. The most frequently used envelope-function method [29] within the Kane–Luttinger model [30] considers that each GaAs and AlAs slab has a band structure close to that of the corresponding bulk crystals and that the band structures of constituent crystals conjugate at interface regions. These approaches can satisfactorily describe only SLs with not too short periods since in the interface region the band description is not valid at all [31].

(ii) The approaches of the second type are called ‘first-principles’ or ‘supercell’ ones and can be applied for both SLs and usual bulk GaAs and AlAs crystals [32]. Only these approaches could be applied to the very short-period SLs. All the first-principles methods use the band approximation. These methods can be classified according to the choice of crystal potential, which is the same for all the electrons of the crystal (method

Table 9. Selection rules for the light absorption in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group D_{2d}^5 (with account of spin-orbit interaction). The labels v and c denote the valence-band and conduction-band virtual states, respectively. $i = 6, 7$; $j = 13 - i$.

Initial state (valence band)	Virtual state	Final state (conduction band)	Assisting phonons	Allowed polarizations
Γ_i	direct transitions	Γ_i Γ_j		x, y $x, y; z$
Γ_i	$\Gamma_{i,c}$	D_5 D_i D_j D_i D_j	$D_1 + D_2 + D_3 + D_4$ $D = R, X$ $D_1 + D_5$ $D = \Gamma, Z$ $D_2 + D_5$ $D = \Gamma, Z$ $D_1 + D_3 + D_5$ $D = M, A$ $D_2 + D_4 + D_5$ $D = M, A$	x, y
Γ_i	$\Gamma_{j,c}$	D_5 D_i D_j D_i D_j	$D_1 + D_2 + D_3 + D_4$ $D = R, X$ $D_2 + D_5$ $D = \Gamma, Z$ $D_1 + D_5$ $D = \Gamma, Z$ $D_2 + D_4 + D_5$ $D = M, A$ $D_1 + D_3 + D_5$ $D = M, A$	$x, y, ; z$
Γ_i	$\Gamma_{i,v}$	Γ_i	$\Gamma_1 + \Gamma_5$	x, y
Γ_i	$\Gamma_{i,v}$	Γ_j	$\Gamma_1 + \Gamma_5$	$x, y; z$
Γ_i	$\Gamma_{j,v}$	Γ_i	$\Gamma_2 + \Gamma_5$	$x, y; z$
Γ_i	$\Gamma_{j,v}$	Γ_j	$\Gamma_2 + \Gamma_5$	x, y

of pseudopotential; local density approximation, LDA; linear muffin-tin-orbital method, LMTO; etc) and according to the choice of basis functions (LCAO or tight-binding; orthogonalized plane waves, OPW; Wannier functions; linearized augmented plane waves, LAPW; etc). Most of them are self-consistent, the form of potential being corrected by an iteration procedure. By analysing these methods one should bear in mind that, if the choice of potential corresponds to different physical models, the difference between LCAO, OPW, or LAPW methods lies in the different choice of basis functions for the expansion of the one-electron eigenfunction. These are atomic orbitals in LCAO, plane waves in OPW, etc. The Wannier function method involves the orbitals constructed from the atomic orbitals of all atoms in the primitive cell.

The calculations of electron-band structures of short-period SLs were performed within both engineering methods (for references see e.g. [20], [21] and [28]) and first-principles approaches [20, 23–27]. We shall try to apply our group-theory results to the recent first-principles band-structure calculations presented in [20], [26] and [27] (LDA), [23] and [25] (pseudopotential), and [24] (LMTO). Though some trends of all the calculations coincide, the comparison of our results with the data of calculations is hindered by the lack of complete symmetry assignment of energy bands in the latter, except for [20] and [26], where the symmetries of uppermost valence-band states and lowest conduction-band ones are given for every SL. The spin-orbit interaction was taken into account only in [23] and [24].

For every short-period SL, the results approximately coincide when the upper valence-band states are considered (the results are summarized in figure 3), the uppermost valence-band state being Γ_6 . The next one has the Γ_7 symmetry. The separations between these states are $\Delta_1 = 21$ meV [24] for the (1×1) SL, and $\Delta_2 = 12$ meV [24] for the (2×2) SL. According to the evaluations of [23] and [24], Δ is approximately the same for all the short-period SLs, varying in the range of 0.1–0.2 eV. The spin-orbit splitting between

Table 10. Selection rules for the light absorption in $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs with the space group D_{2d}^9 (with account of spin-orbit interaction). The labels v and c denote the valence-band and conduction-band virtual states, respectively. $i = 6, 7$; $j = 13 - i$.

Initial state (valence band)	Virtual state	Final state (conduction band)	Assisting phonons		Allowed polarizations
Γ_i	direct transitions	Γ_i			x, y
		Γ_j			$x, y; z$
Γ_i	$\Gamma_{i,c}$	D_i	$D_1 + D_5$	$D = \Gamma, M$	x, y
		D_j	$D_2 + D_5$	$D = \Gamma, M$	
		N_3, N_4	$N_1 + N_2$		
		X_5	$X_1 + X_2 + X_3 + X_4$		
		P_{i-1}	$P_1 + P_3$		
		P_{j-1}	$P_2 + P_4$		
		P_{i+1}	$P_1 + P_4$		
		P_{j+1}	$P_2 + P_3$		
Γ_i	$\Gamma_{j,c}$	D_j	$D_1 + D_5$	$D = \Gamma, M$	$x, y; z$
		D_i	$D_2 + D_5$	$D = \Gamma, M$	
		N_3, N_4	$N_1 + N_2$		
		X_5	$X_1 + X_2 + X_3 + X_4$		
		P_{i-1}	$P_2 + P_4$		
		P_{j-1}	$P_1 + P_3$		
		P_{i+1}	$P_2 + P_3$		
		P_{j+1}	$P_1 + P_4$		
Γ_i	$\Gamma_{i,v}$	Γ_i	$\Gamma_1 + \Gamma_5$		x, y
Γ_i	$\Gamma_{i,v}$	Γ_j	$\Gamma_1 + \Gamma_5$		$x, y; z$
Γ_i	$\Gamma_{j,v}$	Γ_i	$\Gamma_2 + \Gamma_5$		$x, y; z$
Γ_i	$\Gamma_{j,v}$	Γ_j	$\Gamma_2 + \Gamma_5$		x, y

the two (Γ_6 and Γ_7) band states and the lower Γ_7 one is approximately the same as in the case of bulk GaAs, (0.34 ± 0.02) eV [24]. When neglecting the spin-orbit interaction, the uppermost states are Γ_5 and Γ_2 (or Γ_{5v} and Γ_{4v} in the notation of [20], [23] and [26]) with the gap between them being $\Delta_1 = 50$ meV, $\Delta_2 = 20$ meV [20] or even less [23]. Therefore, upon including the spin-orbit interaction, the valence-band state Γ_6 can be considered as derived from the Γ_5 one (section 3), and the Γ_7 state as derived from both Γ_2 and Γ_5 states, provided that the contributions of the remote upper states can be neglected.

The (1×1) SL has an indirect gap according to most of the calculations, the conduction-band minimum being at the R point of the SLBZ (the R_1 state that corresponds to the R_5 state when spin-orbit interaction is included). The calculated band gap is equal to 1.88 eV [20], 1.69 eV [24], 1.85 eV [26], and 1.93 eV [27]. Another minimum is at the M point (the M_5 state). It lies at 2.10 eV [20], 1.92 eV [25], 2.13 eV [26], or 2.12 eV [27]. At the Γ point, the lowest conduction-band state lies higher than the R_1 state by 0.29 eV [20], 0.24 eV [24], 0.26 eV [23], or 0.09 eV [27].

There are essential contradictions between the results of the calculations concerning the ordering in energy of the conduction bands at the Γ point. This results in different optical spectra to be expected. According to [20] and [23] in a (1×1) SL, the Γ_1 state is higher than the Γ_2 state by 10 meV [20] or 300 meV [23]. In [26] a different order was obtained, the lowest conduction-band state being Γ_1 rather than Γ_2 (the latter is 120 meV higher). Unfortunately, none of the calculations takes into consideration the spin-orbit interaction. Since the single-valued representations Γ_1 and Γ_2 correspond, respectively, to the double-

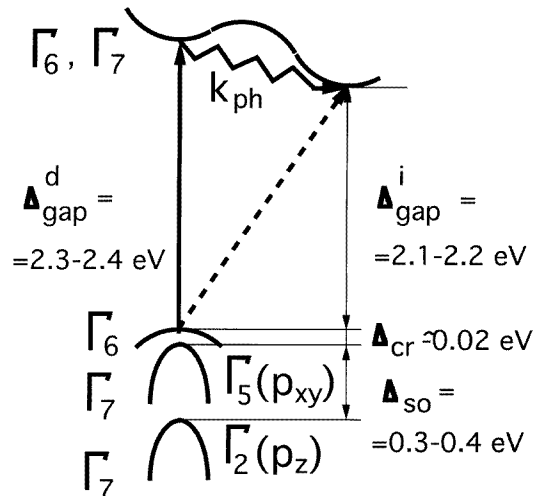


Figure 3. A schematic band-structure diagram of short-period $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs.

valued ones Γ_6 and Γ_7 , it means that the different calculations lead to opposite conclusions concerning the symmetry of the lowest conduction-band Γ state (Γ_6 or Γ_7). Besides, the spin-orbit interaction-induced mixing with lower-lying states may induce energy shifts of the states. In [24], the lowest state at the Γ point in a (1×1) SL is supposed to be Γ_6 as in GaAs and AlAs bulk crystals but without proof of this statement.

This is why we consider two possible energy-level diagrams in the case of (1×1) SL (figure 4) depending on whether the Γ_6 or the Γ_7 conduction-band state is lower. If the lowest conduction-band state has the Γ_7 symmetry, the direct transition with the lowest energy is allowed in every polarization. The two next transitions are forbidden in the z polarization, and, finally, the fourth direct transition with the highest energy is allowed in every polarization. In contrast, if that band state has the Γ_6 symmetry, the first and fourth direct transitions are forbidden in the z polarization, the two others being allowed. In both cases, the transition between the Γ_6 valence-band state (derived from the Γ_5 one) and the Γ_7 conduction-band state (derived from the Γ_2 one) is allowed in the z polarization only on the strength of the spin-orbit interaction, whereas the transition between the Γ_7 valence-band state (originating from both the Γ_2 and Γ_5 ones) and the Γ_6 conduction-band state (derived from the Γ_1 one) is completely allowed (cf table 6). Polarized-absorption experiments could therefore allow us to determine the order of the states.

The phonon-assisted transitions could also provide additional information about the band structure of the (1×1) SL. As a matter of fact, the indirect optical absorption edge corresponds to the transition into the R conduction-band state and is 0.2–0.3 eV lower than the direct one. This should be separated from the so-called ‘indirect’ transitions that may appear due to breaking of the wave-vector-conservation rule by defects, disorder, impurities, interface roughness, etc in actual SLs. Since, at the centre of the BZ, the gap between two uppermost valence-band states is small, it may lead to the appearance of rather weak Γ -phonon-assisted transitions in polarized spectra at the energy positions of forbidden direct transitions. For example, in the case of the uppermost valence-band state and the lowest conduction-band one having the same symmetry Γ_6 (the right part of figure 4), the direct transition is forbidden in the z polarization whereas the $(\Gamma_2 + \Gamma_5)$ -phonon-assisted transition

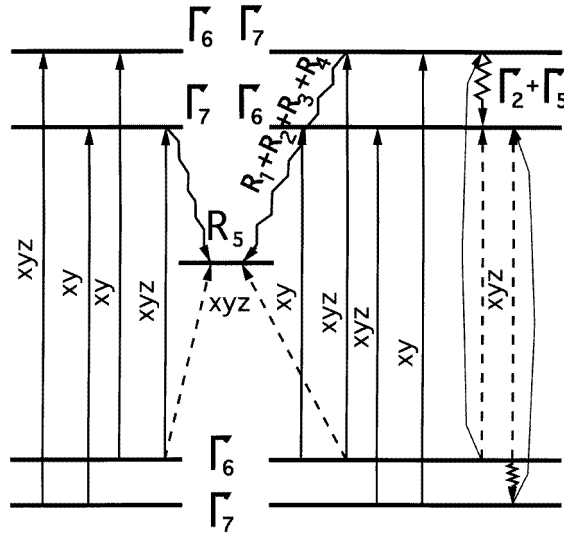


Figure 4. The possible energy-level diagram and dipole-allowed (solid lines) and phonon-assisted (dashed lines) optical transitions in the $(\text{GaAs})_1(\text{AlAs})_1$ [001] SL.

with the same energy is allowed. Moreover, there exist two possible transitions involving either the virtual Γ_7 valence-band state or the virtual Γ_7 conduction-band one (cf table 9). It can be manifest in both absorption and luminescence polarized spectra. One should note that the fine structure of the phonon-assisted transitions is determined not only by the electronic structure but also by the peculiarities of the phonon density of states at the corresponding point of the BZ (the maximal phonon energy is about 50 meV [33]).

The contradictions between the calculations are important in the case of the (2×2) SL. The authors of [20] have obtained that the (2×2) SL has a direct gap with the lowest conduction-band state Γ_1 (Γ_{1c} in their notation) at 2.02 eV, the M_4 state lying 40 meV higher, and the next Γ_1 state lying 210 meV higher. In [24], the lowest state is Γ_6 (the spin-orbit interaction was taken into account) at 2.03 eV. In [25] an M state is also 40 meV higher than the lowest Γ state lying at 1.85 eV. In [26], a different order of the conduction-band states was obtained. According to the calculations of [26], the conduction-band minimum is at the M point of the SLBZ (M_4 state), so this SL has an indirect gap as well as the (1×1) SL. At the Γ point, the lowest conduction-band state is Γ_1 (this corresponds to the results of [20]) but the next Γ_1 state is only 50 meV higher. According to [27], the energy positions of conduction-band minima at the Γ and M points coincide (2.10 eV). Thus, all the calculations give a small difference in energy positions of the lowest Γ_1 (Γ_6) and M_4 (M_7 with spin-orbit interaction included) states in the case of the (2×2) SL.

On analysing a number of experimental data, the authors of [9] and [10] conclude that, for this SL as well as for every $(\text{GaAs})_m(\text{AlAs})_n$ [001]-grown SL with $1 < m, n < 4$, the conduction-band minimum lies at the M point of the SLBZ (folded X_{xy} state in their terminology), a Γ state (folded X_z state) being some tens of meV higher. The authors of [10] note a possible role of the interchange of Ga and Al atoms across the interface, which may result in the essential lowering of the M-state energy.

The calculations give that, for the (2×2) SL, the lowest conduction-band states at the centre of the BZ are the Γ_1 states, the nearest non- Γ_1 state lying as far as 0.5 eV

higher (a Γ_2 state). Provided that the spin-orbit interaction-induced mixing with the remote states is negligible, one can conclude that the lowest conduction-band Γ states have the Γ_6 symmetries. The direct optical transition with the lowest energy is then forbidden in the z polarization, as well as the next one involving the higher-lying Γ_6 state. At the same time, the transitions between the Γ_7 valence-band state and Γ_6 conduction-band ones are completely allowed. The energy-level diagram will be similar to that shown in figure 5. As in the case of the (1×1) SL, there exist Γ -phonon-assisted transitions that make it possible to observe the lowest-energy Γ - Γ optical transition in the z polarization as well. Phonon-assisted indirect optical Γ - M transitions may also be observed; these are weakly allowed in every polarization. Therefore, only a study of the fine structure of the light-absorption spectra of high-quality SLs could allow us to establish the real picture of the interband transitions. Comparing the oscillator strengths of lines in different polarizations one would obtain information on the nature of the lines (direct transitions, phonon-assisted ones) and evaluate the strengths of both spin-orbit and electron-phonon interactions.

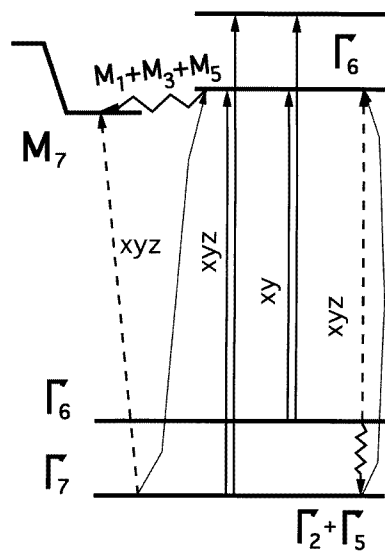


Figure 5. The possible energy-level diagram and dipole-allowed (solid lines) and phonon-assisted (dashed lines) optical transitions in the $(\text{GaAs})_2(\text{AlAs})_2$ [001] SL.

Similar analysis of polarized-light optical spectra could be made in the case of the $(\text{GaAs})_m(\text{AlAs})_n$ SLs with greater m and n .

Summing up, we can say that only experiments could decide in favour of a particular model of band-structure calculations. Nevertheless, when comparing the obtained results with the experimental data one should take into account not only the possible uncertainties arising from the theoretical approximations but also the imperfections of actual SLs. Both the group-theory results and band-structure calculations clearly show that the optical spectra are very sensitive to any variation of SL geometry. The actual structures can differ from the adopted model for different reasons. For example, the lattice-parameter difference between GaAs and AlAs bulk crystals can induce electron energy shifts. This is particularly important if one takes into account the role of the substrate [9]. Besides, the interface roughness can locally vary m and n by one or several units and thereby change the SL symmetry.

5. Conclusion

Summing up, the main results of this paper can be formulated as follows.

(i) The $(\text{GaAs})_m(\text{AlAs})_n$ [001] SLs belong to two crystal families specified by space groups D_{2d}^5 and D_{2d}^9 depending on whether $m + n$ is even or odd. In both cases, there are several subfamilies differing by odd or even numbers of monolayers in both barriers and wells. The main difference between these subfamilies is the interchange of occupation of the same Wyckoff positions by As and Me (Ga, Al) atoms.

(ii) When one goes from one SL to another, the variations of unit-cell geometry resulting in rearrangement of atoms over the Wyckoff positions lead to drastic changes in symmetry of electron and phonon states and in contributions of particular atomic orbitals in the electron states. The latter results in the localization of particular electron bands within either the barriers or the wells. All these changes manifest themselves in optical spectra mainly due to a change of the symmetry of the conduction-band bottom state.

(iii) The selection rules have been derived for both direct and phonon-assisted transitions, the spin-orbit interaction having been taken into account. The latter may be of great importance in short-period SLs. The analysis of the selection rules, results of more reliable band calculations, and the data of polarized-light optical experiments will allow us to create a more precise picture of the electron-band structures of these materials.

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