PHYSICAL REVIEW B VOLUME 61, NUMBER 3 15 JANUARY 2000-I

Bound-state symmetries and optical transitions in GaAs/AlAs quantum wells and superlattices with impurities and defects

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(Received 5 November 1998; revised manuscript received 2 August 1999)

We consider $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ superlattices as single crystals whose structure depends on the growth direction and numbers of monolayers within the slabs of constituent materials. We study point defects such as impurities (substitutional and interstitial) or single vacancies and molecular defects such as paired impurities, double vacancies, or vacancy-impurity complexes in $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ superlattices grown along the [001], [110], and [111] directions. The possible site symmetries of the defects as well as the state symmetries for carriers bound to them have been determined. In contrast to bulk GaAs or AlAs, no defect can present T_d symmetry. The atoms located in the center of the slabs occupy, in most of the [001]- and [110]-grown superlattices, sites with higher symmetries (D_{2d} and C_{2v}, respectively). This results in different selection rules for optical transitions involving the same impurity atom which substitutes the same host atom (Ga, Al, or As) at sites with different symmetries. The effect can be important in optical spectra of superlattices with very thin slabs. The modifications of the selection rules when including the spin-orbit interaction have been derived. Quantum wells can be treated as a particular case of superlattices when barriers become very thick. We present their three-dimensional diperiodic space groups. Quantum wells do not differ from superlattices from the points of view of possible site symmetries and selection rules for optical transitions involving defects. All the above results are also valid for any pseudomorphic superlattice or quantum well made of two binary compounds with zinc-blende structures and identical cations or anions, such as in the GaN/AlN system.

I. INTRODUCTION

The optical properties of semiconductor nanostructures have been extensively studied over the last years. Recently, $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ superlattices (SL's) have been a point of attention.[1–3] We considered SL's as a class of artificially grown crystals whose structure depends on the growth direction and numbers of monolayers within the slabs of constituent materials.[1–3] As a result, we found that, for each direction of growth, SL's constitute several single-crystal families specified by different space groups G_l. Within each family, SL's with different m and n differ from each other by the arrangement of atoms over the Wyckoff positions. Therefore, from the crystallographic point of view, they are distinct crystals. Using the method of induced band representations of space groups,[3] we derived band-to-band optical selection rules for direct and phonon-assisted transitions in SL's with [001], [110], and [111] growth directions. The spin-orbit coupling has been taken into account.[1]

There are only a few papers[4] analyzing impurity states in SL's. Moreover, the authors of Ref. 4 treated them in terms of the parent bulk materials. This approximation is relevant for shallow impurities with rather extended wave functions (mainly donors). On the other hand, deep levels (mainly acceptors) are compact. Their location in the lattice and site symmetry are important. In this paper, we analyze the site symmetry of various crystal defects (CD's), and perform a group-theory study of state symmetries for carriers bound to CD's in SL's grown along the [001], [110], and [111] directions. Finally we derive the optical selection rules for transitions between two states of a CD and between a CD state and a band (extended) state. Although referring below to $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ SL's only, our analysis is valid for any pseudomorphically grown SL made of two binary stoichiometric compounds with zinc-blende structures and identical anions or cations. The atoms in such SL's, are assumed to be on the sites of a zinc-blende lattice, with lattice constant a being an average of the two lattice parameters of parent materials. For $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ SL's taken as the simplest example, the difference in the lattice constants of GaAs and AlAs is less than 0.2%, and the mismatch effects can be neglected whatever is the SL period. When taking this approximation into account, the coordinates of all the atoms in the lattice are uniquely defined. Thus one can determine both the space group and the atomic arrangement over the Wyckoff positions for a perfect SL with arbitrary numbers of monolayers m and n.

The variety of different symmetry (Wyckoff) positions in the primitive cell of the perfect SL's for any atom (Ga, Al, or As) is noticeably larger than in the bulk parent materials.[1–3] In bulk GaAs (AlAs), both metal (Ga or Al) and nonmetal (As) atoms have the same site symmetry T_d. In SL's, metal and nonmetal atoms can in many cases occupy various Wyckoff positions in the primitive cell depending both on the growth direction and the number of monolayers. This results in different behaviors of the same impurity atom, which substitutes for the same host atom (Ga, Al, or As) at sites with different symmetries.

0163-1829/2000/61(3)/1999(9)/$15.00

TABLE I. Possible occupation numbers (per primitive cell) for substitutional CD's in the $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ superlattices.

Atoms substituted	Site symmetry	Growth direction and space group									
			[001]				[110]			[111]	
			D_{2d}^5		D_{2d}^9	C_{2v}^1	C_{2v}^7		C_{2v}^{20}	C_{3v}^1	C_{3v}^5
		$m=2k+1$	$m=2k$	$m=2k+1$	$m=2k$	$m=2k+1$	$m=2k$	$m=2k+1$	$m=2k$	$m+n=3k$	$m+n\neq 3k$
		$n=2s+1$	$n=2s$	$n=2s$	$n=2s+1$	$n=2s+1$	$n=2s$	$n=2s$	$n=2s+1$		
Ga	D_{2d}	1	-	1	-	-	-	-	-	-	-
	C_{2v}	$m-1$	m	$m-1$	m	1	-	1	-	-	-
	C_{3v}	-	-	-	-	-	-	-	-	m	m
	C_s	-	-	-	-	$m-1$	m	$m-1$	m	-	-
Al	D_{2d}	1	-	-	1	-	-	-	-	-	-
	C_{2v}	$n-1$	n	n	$n-1$	1	-	-	1	-	-
	C_{3v}	-	-	-	-	-	-	-	-	n	n
	C_s	-	-	-	-	$n-1$	n	n	$n-1$	-	-
As	D_{2d}	-	2	1	1	-	-	-	-	-	-
	C_{2v}	$m+n$	$m+n-2$	$m+n-1$	$m+n-1$	2	-	1	1	-	-
	C_{3v}	-	-	-	-	-	-	-	-	$m+n$	$m+n$
	C_s	-	-	-	-	$m+n-2$	$m+n$	$m+n-1$	$m+n-1$	-	-
Ga(Al)+As	C_{3v}	-	-	-	-	-	-	-	-	$m(n)$	$m(n)$
	C_s	$4m(n)$	$4m(n)$	$4m(n)$	$4m(n)$	$2m(n)$	$2m(n)$	$2m(n)$	$2m(n)$	$3m(n)$	$3m(n)$
	C_1	-	-	-	-	$2m(n)$	$2m(n)$	$2m(n)$	$2m(n)$	-	-

The aim of this paper is to show how the distribution of impurities and defects over the Wyckoff positions manifest themselves in polarized optical spectra, and, conversely, how one can obtain information from the spectra, e.g., about the sites of dopants in the lattice. In Sec. II, we analyze the nature and symmetry of various CD's. In Sec. III, we derive the selection rules for optical transitions involving CD states, and discuss the peculiarities in the polarized spectra which could be observed. In Sec. IV, we extend our results to GaAs/AlAs quantum wells (QW's). In Sec. V, we discuss some experimental data available in the literature, and propose an interpretation in terms of the present analysis.

II. CLASSIFICATION OF CRYSTAL DEFECTS AND THEIR SITE SYMMETRIES IN SL's

We pay attention to point CD's such as vacancies, substitutional and interstitial impurities, and molecular defects (paired impurities, double vacancies, and vacancy-impurity complexes), but do not consider the defects of the SL structure which result from the imperfections of various growth techniques: fluctuations of the thicknesses of the constituent semiconductor layers, dislocations, roughness of interfaces, etc. We assume that the site-symmetry group G_q is not modified when a SL atom in position q is replaced by a substitutional impurity or by a single vacancy. The same assumption is made for an interstitial impurity. As a consequence, the Hamiltonian of a carrier bound to the defect has the symmetry of the site in the perfect crystal.

A. Substitutional impurities and vacancies

Possible occupation numbers per primitive cell for substitutional impurities or single vacancies in SL's grown along different directions are given in Table I. As an example, two [001] SL's are illustrated in Fig. 1. One can see that Ga and Al atoms occupy D_{2d} sites, and As atoms occupy C_{2v} sites in the $(\mathrm{GaAs})_1(\mathrm{AlAs})_1$ [001]-grown SL, whereas in the $(\mathrm{GaAs})_2(\mathrm{AlAs})_2$ [001] SL, the metal (Ga, Al) atoms occupy C_{2v} sites and As atoms are distributed among the D_{2d} and C_{2v} sites. If a CD substitutes for a metal atom in these two SL's, the optical transitions involving this impurity are different. Moreover, the behavior of impurities substituting for As atoms at sites with different symmetries in the 2×2 SL, will also be different. Thus provides a possibility to determine the sites of dopants in the lattice when analyzing the optical spectra.

B. Interstitial impurities

Interstitial impurities can be classified into three types according to the Wyckoff position they occupy. Those of the first type occupy the same Wyckoff positions as atoms of the SL. This is possible if the Wyckoff positions are not isolated points but symmetry lines, symmetry planes, or continuous three-dimensional sets of symmetry points. In this case, the substitutional and interstitial impurities have no difference in behavior from the point of view of symmetry. The interstitial impurities of the second type occupy those unoccupied Wyckoff positions which have the same site symmetry as those occupied by atoms of the SL. In this case, the substitutional and interstitial impurities have no difference in symmetry behavior for optical transitions involving only the Γ-point band states (see Sec. III). Finally, there may exist Wyckoff positions which are not occupied by atoms in the lattice, and which have different site symmetry than the occupied ones. These sites have C_1 symmetry (i.e., no symmetry) for all SL's in question except for the [001] SL's, where C_2 sites also exist. The Wyckoff positions with C_1 symmetry are the three-dimensional sets.

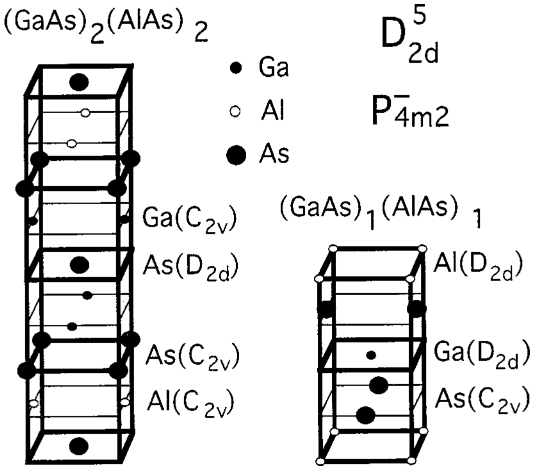

FIG. 1. Possible symmetry sites for substitutional CD’s in the $(GaAs)_1(AlAs)_1$ and $(GaAs)_2(AlAs)_2$ [001] SL’s.

Below, for all SL’s, we list the sets of Wyckoff positions and their symmetries as well as types of CD (substitutional *s* and interstitial *i*) which can occupy these positions:

D_{2d}^5: D_{2d}-$1a(s)$, $1b(i)$, $1c(s \text{ or } i)$, $1d(s \text{ or } i)$; C_{2v} $-\underline{2e}(s \text{ and } i)$, $\underline{2f}(s \text{ and } i)$, $\underline{2g}(s \text{ and } i)$; C_s—$\underline{\underline{4j}}(i)$, $\underline{\underline{4k}}(i)$; C_2—$\underline{4h}(i)$, $\underline{4i}(i)$; C_1—$\underline{\underline{\underline{8l}}}(i)$.

D_{2d}^9: D_{2d}-$1a(s)$, $1b(i)$, $1c(s \text{ or } i)$, $1d(s \text{ or } i)$; C_{2v}—$\underline{2e}(s \text{ and } i)$, $\underline{2f}(s \text{ and } i)$; C_s—$\underline{\underline{4i}}(i)$; $C_2-\underline{4g}(i)$, $\underline{4h}(i)$; C_1—$\underline{\underline{\underline{8j}}}(i)$.

C_{2v}^1: C_{2v}-$\underline{1a}(s \text{ and } i)$, $\underline{1b}(s \text{ and } i)$, $\underline{1c}(s \text{ and } i)$, $\underline{1d}(s \text{ and } i)$; $C_s(\sigma_x)$—$\underline{\underline{2g}}(s \text{ and } i)$, $\underline{\underline{2h}}(i)$; $C_s(\sigma_y)$—$\underline{\underline{2e}}(i)$, $\underline{\underline{2f}}(i)$; C_1—$\underline{\underline{\underline{4i}}}(i)$.

C_{2v}^7: $C_s(\sigma_x)$-$\underline{\underline{2a}}(s \text{ and } i)$; C_1—$\underline{\underline{\underline{4b}}}(i)$.

C_{2v}^{20}: C_{2v}-$\underline{1a}(s \text{ and } i)$, $\underline{1b}(s \text{ and } i)$; $C_s(\sigma_y)$—$\underline{\underline{2c}}(i)$; $C_s(\sigma_x)$—$\underline{\underline{2d}}(s \text{ and } i)$; C_1—$\underline{\underline{\underline{4e}}}(i)$.

C_{3v}^1: C_{3v}-$\underline{1a}(s \text{ and } i)$, $\underline{1b}(s \text{ and } i)$, $\underline{1c}(s \text{ and } i)$; C_s—$\underline{\underline{3d}}(i)$; C_1—$\underline{\underline{\underline{6e}}}(i)$.

C_{3v}^5: C_{3v}-$\underline{1a}(s \text{ and } i)$; C_s—$\underline{\underline{3b}}(i)$; C_1—$\underline{\underline{\underline{6c}}}(i)$.

In the list above, Wyckoff positions which are not underlined are isolated symmetry points. Those which are underlined once are symmetry lines, those underlined twice are symmetry planes, and those underlined three times are three-dimensional sets. The symmetry planes and most of the symmetry lines are parallel to the symmetry (growth) axis. For more details, see Ref. 5. As already mentioned, the Wyckoff positions which are symmetry lines, symmetry planes, or three-dimensional sets can be occupied either by substitutional and interstitial CD’s or by interstitial ones only. The position being isolated symmetry points can be occupied either by substitutional or interstitial CD’s, depending on whether this position is occupied or not by an atom in a particular SL.

C. Molecular CD’s

We consider molecular CD’s occupying two atomic or interstitial sites. The symmetry group of such a CD is determined by the common elements of two groups: the point group of the isolated «molecule» whose axis coincides with the line connecting the two involved SL sites ($C_{\infty v}$ or $D_{\infty h}$), and the site-symmetry group of any point on this line between both sites (C_{nv}, D_{nh}, D_{nd}, C_n, C_s, or C_1). The distribution over the Wyckoff positions of possible molecular CD’s involving two nearest-neighbor atomic sites of the SL is presented in Table I. All of them have the same C_s site symmetry in [001]-grown SL’s. Obviously, they may have different energies. If they were randomly distributed over the atomic sites, the ratio between the numbers of (Ga+As) and (Al+As) complexes would be $m:n$. The same ratio holds in [110]- and [111]-grown SL’s. Half of such possible complexes in [110] SL’s would have the lowest C_1-site symmetry. In [111] SL’s, the ratio between higher-symmetry (C_{3v}) molecular CD’s and lower-symmetry (C_s) ones is 1:3. This can be seen simply in Fig. 2, where the C_{3v} complex is distinguished. Further, the displacement of single CD’s within the molecular ones is of importance. It is remarkable that, for a molecular CD which is located at places of two nearest-neighboring atoms, the displacements of the components along the line connecting them does not alter the CD symmetry group for any SL, although it changes the energy. This can considerably simplify the symmetry analysis of molecular CD’s (for bulk GaAs, the molecular CD-energy dependence on the displacement of a CD component from the initial position into the [111] direction was studied in Refs. 6 and 7, in particular the (V_{As},As_{Ga}) pair[7]).

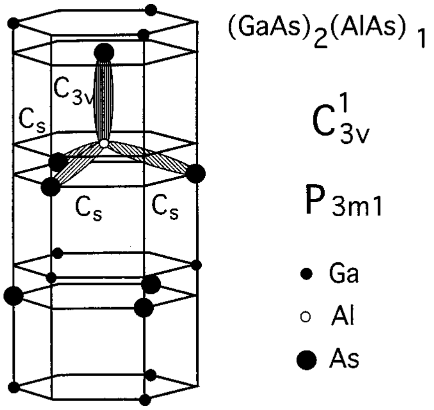

FIG. 2. Orientations and site symmetries of paired crystal defects involving the nearest neighbors in the $(GaAs)_2(AlAs)_1$ [111]-grown SL.

Summing up, being T_d in the bulk parent materials, the site-symmetry group G_q for point defects is lowered in the SL’s down to D_{2d}, C_{2v}, C_{3v}, C_s, or even C_1 (only for interstitial CD’s) depending on the occupied Wyckoff position, growth direction, and number of monolayers. For molecular CD’s, the symmetry is lowered from C_{3v} down to C_s or C_1. It is worth noting that no CD presents T_d symmetry. Most of the atoms of the lattice occupy sites with C_{2v}, C_s, and C_{3v} symmetry for [001], [110], and [111] growth direction, respectively. In all SL’s grown along the [001] and [110] directions except those with the C_{2v}^7 space group (Table I), there are few (two or four) atoms per primitive cell with a higher site symmetry (D_{2d} and C_{2v}, respectively). These atoms are those located at the center of the slabs. The effect on optical spectra of CD’s located at the latter sites can be important for SL’s with very thin slabs.

III. OPTICAL SELECTION RULES

Let the symmetry of a CD localized state be described by the irrep d_α of the CD site-symmetry group G_q and the sym-

TABLE II. The selection rules for direct transitions between a CD state and a Γ-band state in [001]-grown SL's (the space groups D_{2d}^5,D_{2d}^9) and QW's (the space group DG59). The labels of the irreps taken in brackets refer to the case where spin-orbit coupling is not taken into account. Polarizations in brackets (parentheses) refer to transitions allowed only without (with) including spin-orbit interaction; the ones in capitals refer to the transitions allowed in both cases. Corep: $\overline{e}^{(1)}+\overline{e}^{(2)}$. The X' and Y' axes are rotated 45° along the Z axis with respect to the X and Y axes.

CD site	Localized state	Conduction (valence) band state			
		$\Gamma_6\ [\Gamma_1]$	$\Gamma_7\ [\Gamma_2]$	$\Gamma_6\ [\Gamma_5]$	$\Gamma_7\ [\Gamma_5]$
D_{2d}	$\overline{e_1}[a_1(s;d_{z^2})]$	(x,y)	$(x,y)Z$	X,Y	$X,Y(z)$
	$\overline{e_2}[b_1(d_{x^2y^2})]$	(x,y,z)	(x,y)	$X,Y(z)$	X,Y
	$\overline{e_2}[b_2(p_{zi};d_{xy})]$	$(x,y)Z$	(x,y)	$X,Y(z)$	X,Y
	$\overline{e_1}[e(p_x,p_y;d_{yz},d_{xz})]$	(X,Y)	$X,Y(z)$	$(x,y)[z]$	$(x,y)Z$
	$\overline{e_2}[e(p_x,p_y;d_{yz},d_{xz})]$	$X,Y(z)$	X,Y	$(x,y)Z$	$(x,y)[z]$
C_{2v}	$\overline{e}[a_1(s;p_z;d_{x^2};d_{y^2};d_{z^2})]$	$(x,y)Z$	$(x,y)Z$	$X,Y(z)$	$X,Y(z)$
	$\overline{e}[a_2(d_{xy})]$	(x,y,z)	(x,y,z)	$X,Y(z)$	$X,Y(z)$
	$\overline{e}[b_1(p_{xj};d_{xz})]$	$X(y,z)$	$X(y,z)$	$(x,y)Z$	$(x,y)Z$
	$\overline{e}[b_2(p_y;d_{yz})]$	$Y(x,z)$	$Y(x,z)$	$(x,y)Z$	$(x,y)Z$
$C_S(\sigma_x)$	$\overline{e}^{(1),(2)}[a'(s;p_y;p_z;d_{x^2};d_{y^2};d_{z^2};d_{yz})]$	$(x)Y,Z$	$X(y,z)$	X,Y,Z	X,Y,Z
	$\overline{e}^{(1),(2)}[a''(p_x;d_{xz};d_{xy})]$	$X(y,z)$	$(x)Y,Z$	X,Y,Z	X,Y,Z
$C_S(\sigma_y)$	$\overline{e}^{(1),(2)}[a'(s;p_x;p_z;d_{x^2};d_{y^2};d_{z^2};d_{xz})]$	$(y)X,Z$	$Y(x,z)$	X,Y,Z	X,Y,Z
	$\overline{e}^{(1),(2)}[a''(p_y;d_{yz};d_{xy})]$	$Y(x,z)$	$(y)X,Z$	X,Y,Z	X,Y,Z
C_S(av)	$\overline{e}^{(1),(2)}[a']$	X,Y,Z	$X,Y(z)$	X,Y,Z	X,Y,Z
	$\overline{e}^{(1),(2)}[a'']$	$X,Y(z)$	X,Y,Z	X,Y,Z	X,Y,Z
C_2	$\overline{e}^{(1),(2)}[a(s;p_{x'};d_{x'^2};d_{y'^2};d_{z^2};d_{y'z})]$	$X'(y',z)$	$(x')Y',Z$	X',Y',Z	X',Y',Z
(U_{xy})	$\overline{e}^{(1),(2)}[b(p_{y'};p_z;d_{x'y'};d_{x'z})]$	$(x')Y',Z$	$X'(y',z)$	X',Y',Z	X',Y',Z
C_2	$\overline{e}^{(1),(2)}[a(s;p_{y'};d_{x'^2};d_{y'^2};d_{z^2};d_{x'z})]$	$Y'(x',z)$	$(y')X',Z$	X',Y',Z	X',Y',Z
$(U_{\overline{xy}})$	$\overline{e}^{(1),(2)}[b(p_{x'};p_z;d_{x'y'};d_{y'z})]$	$(y')X',Z$	$Y'(x',z)$	X',Y',Z	X',Y',Z
C_2(av)	$\overline{e}^{(1),(2)}[a]$	$X,Y(z)$	X,Y,Z	X,Y,Z	X,Y,Z
	$\overline{e}^{(1),(2)}[b]$	X,Y,Z	$X,Y(z)$	X,Y,Z	X,Y,Z

metry of an electron state in a conduction or valence band of the SL by the irrep D_β of the SL space group G. To determine the allowed direct transitions between the d_α and D_β states, one should subduce[3] the irrep D_β on the site symmetry group G_q:

$$D_\beta \downarrow G_q = \sum_\gamma A_\gamma d_\gamma. \tag{1}$$

The transition between the d_α and D_β states is allowed if

$$(D_\beta \downarrow G_q)^* \times d_\alpha \cap d_v \neq 0, \tag{2}$$

where d_v is the vector representation of the site-symmetry group G_q. The vector representation is $b_2(z)+e(x,y)$, $a_1(z)+b_1(x)+b_2(y)$, $a_1(z)+e(x,y)$, $a'(u,v)+a''(z)$, for D_{2d}, C_{2v}, C_{3v}, C_s and C_2 and $a(u')+b(v',z)$ site-symmetry groups, respectively (U and V axes being parallel and perpendicular to the mirror plane, respectively, U'being along the twofold rotation axis). Transitions between the d_α and d_β states of a CD, that is to say ''intra-CD'' transitions, are allowed if

$$(d_\alpha)^* \times d_\beta \cap d_v \neq 0. \tag{3}$$

Reversing time obviously does not modify the selection rules. For $\mathbf{k}=0$ band states, the result of subduction [see Eq. (1)] depends only on the point group of the site. However, when subducing the irreps of $\mathbf{k}\neq 0$ band states, one should specify the Wyckoff position, since the groups of different sites (even with the same point group) contain different translations which contribute into Eq. (1) when $\mathbf{k}\neq 0$. Among the bound states, those described by two-dimensional irreps are of a special interest. The degeneracy of these states can be lifted by external perturbation, e.g., by a magnetic or electric field, thus multiplying the number of transitions in the spectra. When the spin-orbit interaction is taken into account the initial and final states in Eqs. (1)–(3) are described by double-valued irreps. In this case, the selection rules are modified, and some forbidden transitions become allowed whereas some allowed transitions become forbidden.

Tables II–IV display the selection rules for transitions between localized and SL Γ states as well as the modification of the selection rules upon including spin-orbit interaction. We consider not only *s* and *p* states but also *d* states since the latter orbitals correspond to the upper occupied states in, for example, transition metals. We do not specify the explicit form of the localized CD functions. Their spatial distributions within the primitive cell remain undefined in

TABLE III. The selection rules for direct transitions between a CD state and a Γ-band state in [110]-grown SL's (the space groups C_{2v}^1, C_{2v}^7, and C_{2v}^{20}) and QW's (the space groups DG24 and DG32). The notations are the same as in Table II. Corep: $\overline{e}^{(1)}+\overline{e}^{(2)}$.

CD site	Localized state	Conduction (valence) band state			
		Γ_5 $[\Gamma_1]$	Γ_5 $[\Gamma_2]$	Γ_5 $[\Gamma_3]$	Γ_5 $[\Gamma_4]$
C_{2v}	$\overline{e}[a_1(s;p_z;d_{x^2};d_{y^2};d_{z^2})]$	$(x,y)Z$	(x,y,z)	$Y(x,z)$	$X(y,z)$
	$\overline{e}[a_2(d_{xy})]$	(x,y,z)	$(x,y)Z$	$X(y,z)$	$Y(x,z)$
	$\overline{e}[b_1(p_x;d_{xz})]$	$X(y,z)$	$Y(x,z)$	(x,y,z)	$(x,y)Z$
	$\overline{e}[b_2(p_y;d_{yz})]$	$Y(x,z)$	$X(y,z)$	$(x,y)Z$	(x,y,z)
$C_s(\sigma_x)$	$\overline{e}^{(1),(2)}[a'(s;p_y;p_z;d_{x^2};d_{y^2};d_{z^2};d_{yz})]$	$(x)Y,Z$	$X(y,Z)$	$(x)Y,Z$	$X(y,z)$
	$\overline{e}^{(1),(2)}[a''(p_x;d_{xz};d_{xy})]$	$X(y,z)$	$(x)Y,Z$	$X(y,z)$	$(x)Y,Z$
$C_s(\sigma_y)$	$\overline{e}^{(1),(2)}[a'(s;p_x;p_z;d_{x^2};d_{y^2};d_{z^2};d_{xz})]$	$(y)X,Z$	$Y(x,z)$	$(y)X,Z$	$Y(x,z)$
	$\overline{e}^{(1),(2)}[a''(p_y;d_{yz};d_{xy})]$	$Y(x,z)$	$(y)X,Z$	$Y(x,z)$	$(y)X,Z$

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 different sites belonging to the same orbit can have site-symmetry groups differently oriented with respect to *x*, *y*, and *z* axes.[3] In general, the symmetry groups G_{q_i} and G_{q_j} of sites $\mathbf{q}_i$ and $\mathbf{q}_j$ transforming into each other by the element g_{ij} ($\mathbf{q}_j = g_{ij}\mathbf{q}_j$) are connected by the relation $G_{q_j} = g_{ij} G_{q_i} g_{ij}^{-1}$. For example, in SL's with D_{2d}^5 symmetry, the orbit belonging to the $4j$ Wyckoff position contains four sites $(0\,y\,z)$, $(0-y\,z)$, $(y\,0-z)$, and $(-y\,0-z)$. The first pair has site symmetry C_s with a σ_x mirror plane, whereas the site symmetry of the second pair is C_s with a σ_y mirror plane. The optical selection rules for the second pair can be directly obtained from the rules for the first one by permutation of *x* and *y* coordinates. For orbits containing positions with different orientations of site-symmetry groups, we also present, when all positions in the orbit are randomly occupied, the selection rules obtained by summation of contributions of all positions in the orbit. In this case, we do not specify the localized functions and mark these cases in Tables II–IV as average (av). On the other hand, in SL's with C_{2v}^1 symmetry, both sites $(0\,y\,z)$ and $(0-y\,z)$ in the orbit belonging to the $2g$ Wyckoff position (as well as to the $2h$ one) have site symmetry C_s with a σ_x mirror plane, whereas all the sites in orbits belonging to the $2e$ and $2\,f$ positions have site symmetry C_s with a σ_y mirror plane. Therefore, in this case the states with σ_x and σ_y symmetries can be distinguished in optical spectra. The results given in Tables II–IV are valid for any CD.

Note that the labeling of the symmetry sites is given according to Ref. 5. All the coordinates are given in units of translation vectors of the corresponding crystallographic unit cell (tetragonal, orthorhombic, and hexagonal, respectively). To keep the standard settings of space groups for [110]-grown SL's, the *y* axis is chosen to be the growth direction in contrast to [001]- and [111]-grown SL's where it is the *z* axis. In addition, in [111] SL's the angle between the *x* and *y* axes is 120°. The labeling of point-group irreps follows Ref.

TABLE IV. The selection rules for direct transitions between a CD state and a Γ-band state in [111]-grown SL's (the space groups C_{3v}^1 and C_{3v}^5) and QW's (the space group DG69). The notations are the same as in Table II. Coreps: $\Gamma_4+\Gamma_5$, $\overline{e}_1^{(1)}+\overline{e}_1^{(2)}$, and $\overline{e}^{(1)}+\overline{e}^{(2)}$. The angle between the *U* and *V* axes is 90°, with the *V* axis being prependicular to the symmetry plane of C_s site group (there are three sites in this orbit).

CD site	Localized state	Conduction (valence) band state			
		$\Gamma_4\,[\Gamma_3]$	$\Gamma_5\,[\Gamma_3]$	$\Gamma_6\,[\Gamma_1]$	$\Gamma_6\,[\Gamma_3]$
C_{3v}	$\overline{e}_1^{(1)}[e(p_x,p_y;d_{x^2y^2},d_{xy};d_{xz},d_{yz})]$	$[x,y]Z$	$[x,y,z]$	X,Y	$X,Y[z]$
	$\overline{e}_1^{(2)}[e(p_x,p_y;d_{x^2y^2},d_{xy};d_{xz},d_{yz})]$	$[x,y,z]$	$[x,y]Z$	X,Y	$X,Y[z]$
	$\overline{e_2}[a_1(s;p_z;d_{z^2})]$	X,Y	X,Y	$(x,y)Z$	$X,Y(z)$
	$\overline{e_2}[e(p_x,p_y;d_{x^2-y^2},d_{xy};d_{xz},d_{yz})]$	$X,Y[z]$	$X,Y[z]$	$X,Y(z)$	X,Y,Z
C_S	$\overline{e}^{(1)}[a'(s;p_u;p_z;d_{u^2};d_{v^2};d_{z^2};d_{uz})]$	$U,Z[v]$	$V[u,z]$	$U,Z(v)$	U,V,Z
	$\overline{e}^{(1)}[a''(p_v;d_{vz};d_{uv})]$	$U,Z[v]$	$V[u,z]$	$V(u,z)$	U,V,Z
	$\overline{e}^{(2)}[a'(s;p_u;p_z;d_{u^2};d_{v^2};d_{z^2};d_{uz})]$	$V[u,z]$	$U,Z[v]$	$U,Z(v)$	U,V,Z
	$\overline{e}^{(2)}[a''(p_v;d_{vz};d_{uv})]$	$V[u,z]$	$U,Z[v]$	$V(u,z)$	U,V,Z
C_S(av)	$\overline{e}^{(1)}[a']$	X,Y,Z	$X,Y[z]$	X,Y,Z	X,Y,Z
	$\overline{e}^{(1)}[a'']$	X,Y,Z	$X,Y[z]$	$X,Y(z)$	X,Y,Z
	$\overline{e}^{(2)}[a']$	$X,Y[z]$	X,Y,Z	X,Y,Z	X,Y,Z
	$\overline{e}^{(2)}[a'']$	$X,Y[z]$	X,Y,Z	$X,Y(z)$	X,Y,Z

TABLE V. The possible states of a CD, displayed along the first row and first column of each block. Kronecker products of states are given together with the allowed polarizations for optical transitions, in parentheses, provided by each term of the products. Coreps: $\overline{e}^{(1)}+\overline{e}^{(2)}$ and $\overline{e}_1^{(1)}+\overline{e}_1^{(2)}$.

CD site	CD-state Kronecker products ($d_\alpha^* \times d_\beta$) and allowed polarizations				
		Neglecting spin-orbit interaction			
D_{2d}		a_1	b_1	b_2	e
	a_1	a_1	b_1	$b_2(z)$	$e(x,y)$
	b_1	b_1	a_1	a_2	$e(x,y)$
	b_2	$b_2(z)$	a_2	a_1	$e(x,y)$
	e	$e(x,y)$	$e(x,y)$	$e(x,y)$	$a_1+a_2+b_1+b_2(z)$
C_{2v}		a_1	a_2	b_1	b_2
	a_1	$a_1(z)$	a_2	$b_1(x)$	$b_2(y)$
	a_2	a_2	$a_1(z)$	$b_2(y)$	$b_1(x)$
	b_1	$b_1(x)$	$b_2(y)$	$a_1(z)$	a_2
	b_2	$b_2(y)$	$b_1(x)$	a_2	$a_1(z)$
C_{3v}		a_1	e		
	a_1	$a_1(z)$	$e(x,y)$		
	e_2	$e(x,y)$	$a_1(z)+a_2+e(x,y)$		
$C_S(\sigma_x)$		a'	a''		
	a'	$a'(y,z)$	$a''(x)$		
	a''	$a''(x)$	$a'(y,z)$		
		Taking into account spin-orbit interaction			
D_{2d}		$\overline{e_1}$	$\overline{e_2}$		
	$\overline{e_1}$	$a_1+a_2+e(x,y)$	$b_1+b_2(z)+e(x,y)$		
	$\overline{e_2}$	$b_1+b_2(z)+e(x,y)$	$a_1+a_2+e(x,y)$		
C_{2v}		$\overline{e}$			
	$\overline{e}$	$a_1(z)+a_2+b_1(x)+b_2(y)$			
C_{3v}		$\overline{e}_1^{(1)}$	$e_1^{(2)}$	$\overline{e_2}$	
	$\overline{e}_1^{(1)}$	$a_1(z)$	a_2	$e(x,y)$	
	$\overline{e}_1^{(2)}$	a_2	$a_1(z)$	$e(x,y)$	
	$\overline{e_2}$	$e(x,y)$	$e(x,y)$	$a_1(z)+a_2+e(x,y)$	
$C_S(\sigma_x)$		$\overline{e}^{(1)}$	$\overline{e}^{(2)}$		
	$\overline{e}^{(1)}$	$a'(y,z)$	$a''(x)$		
	$\overline{e}^{(2)}$	$a''(x)$	$a'(y,z)$		

8; the irreps of the space groups are labeled according to Ref. 9. Some of the irreps in Tables II–IV are complex conjugated. Two such irreps form a pair and correspond to two different states with the same energy. This degeneracy is connected with the inversion of time, and can be lifted by applying a magnetic field, which does not reduce the point symmetry of the system (that is a field parallel to the symmetry axis). The complex-conjugated irreps can be combined in so-called corepresentations (coreps). The corresponding pairs of irreps forming coreps are given in the captions of Tables II–IV. On applying the magnetic field, the states described by complex-conjugated irreps are split, whereas states described by doubly degenerate irreps are not.

A similar analysis can be performed for intra-CD transitions. [To our knowledge, there is only one paper[10] devoted to the study of intra-CD transitions in SL's like $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$. The behavior of the transition between the $1s$-$2p$ donor states was investigated for rather long-period GaAs/Ga$_{1-x}$Al$_x$As SL's] Table V gives selection rules for intra-CD transitions when neglecting and including the spin-orbit interaction. Upon including the spin-orbit interaction, there exists only one doubly degenerate irrep $\overline{e}$ of the C_{2v} site-symmetry group, and every transition becomes allowed in every polarization. In the case of the C_s site symmetry, when spin-orbit coupling is taken into account, every state is also described by the same corep $\overline{e}^{(1)}+\overline{e}^{(2)}$, but splits on applying a magnetic field along the growth direction. More complicated is the case of the C_{3v} site symmetry. When spin-orbit coupling is included, there are states that are described by the doubly degenerate irrep $\overline{e_2}$ as well as states which can be described by the corep $\overline{e}_1^{(1)}+\overline{e}_1^{(2)}$. Only the latter splits on applying a magnetic field along the growth direction. Note that for the CD's with C_{3v} site symmetry, there are two kinds of doubly degenerate $\overline{e_2}$ states, originating from the a_1 state and the doubly degenerate e state, respectively.

TABLE VI. Possible occupation numbers (per primitive cell) for substitutional CD's in AlAs/GaAs/AlAs quantum wells.

		Growth direction and diperiodic space group (DG)				
		[001] DG 59 ($P\bar{4}m2$)		[110] DG 24 ($Pmm2$)	DG 32 ($Pnm2_1$)	[111] DG 69 ($P3m1$)
Atoms substituted	Site symmetry	$m=2k+1$	$m=2k$	$m=2k+1$	$m=2k$	
Ga	D_{2d}	1	-	-	-	-
	C_{2v}	$m-1$	m	1	-	-
	C_{3v}	-	-	-	-	m
	C_s	-	-	$m-1$	m	-
As	D_{2d}	-	1	-	-	-
	C_{2v}	m	$m-1$	1	-	-
	C_{3v}	-	-	-	-	m
	C_s	-	-	$m-1$	m	-
Ga-As	C_{3v}	-	-	-	-	m
	C_s	$4m$	$4m$	$2m$	$2m$	$3m$
	C_1	-	-	$2m$	$2m$	-

In addition to transitions involving band states at the center of the Brillouin zone, those involving band states with $k \neq 0$ may be of importance. The momentum conservation in transitions involving CD-localized states does not imply wave-vector conservation in these processes. Though above we considered only transitions between localized states and Γ states, one can easily obtain the corresponding selection rules for transitions involving band states with $k \neq 0$ without participation of phonons. As previously performed for the Γ states, one should subduce the corresponding irrep on the site-symmetry group. However, in the $k \neq 0$ case one should specify not only the point group of the site but also the position itself.[1] For a SL with a D_{2d}^5 space group taken as an example, the transition between M_2 and a_1 is allowed in the z polarization for the CD substituting an atom at the $1a$ site, whereas for the $1c$ site the z-allowed transition is between M_3 and a_1.

IV. QUANTUM WELLS

QW's may be treated as a particular case of a SL with a barrier thickness going to infinity or, at least, becoming large enough to prevent tunneling of carriers between wells. The minimal thickness of a barrier to achieve such a situation is of the order of a few tens of monolayers. For holes, the well material is GaAs in any case, whereas, for electrons, it is either GaAs or AlAs depending on whether the heterostructure is type I or type II.[11] Here we assume that the well material is GaAs. An identical picture would be obtained with AlAs just by replacing m by n.

When transforming from a $(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ SL to a single QW, the point-group symmetry remains the same, whereas the space group changes from a three-dimensional (3D) triperiodic one to a 3D diperiodic group (DG) or layer group[12] since the translational invariance along the z axis is lost. (Notice that for QW's the growth direction is always along the z axis). We present three-dimensional diperiodic groups for single QW's in Table VI. The diperiodic space group of a QW does not depend on the manner in which the barrier goes to infinity, though the intermediate structures could have different symmetries depending on the widths of the barrier (even or odd values of n). Indeed, Table VI shows that the diperiodic space group of the QW depends only on the parity of m for the [110] growth direction, and only on growth direction for the [001] and [111] growth directions.

Considering CD's of the same nature as those we studied above in SL's, from Table I we deduce the possible occupation numbers for substitutional CD's in AlAs/GaAs/AlAs QW's (Table VI). As in SL's, most of the atoms of the lattice occupy sites with C_{2v}, C_s, and C_{3v} symmetry for [001], [110], and [111] growth directions, respectively. In all QW's grown along the [001] and [110] directions, except those with the DG 32 ($Pnm2_1$) space group, there is (are) one (or two) atom(s) with a higher site symmetry (D_{2d} and C_{2v}, respectively). These atoms are those located at the center of the QW's. The possible site symmetries for CD's within the wells therefore are the same as in SL's, which allows one to conclude that the intra-CD optical selection rules remain the same (Table V).

Below, in the same manner as for SL's, for all QW's we give the sets of Wyckoff positions together with their symmetries as well as types of CD which can occupy these positions (all notations are as given above). The diperiodic groups and their Wyckoff position labeling follow the notations of Wood[12]:

DG 59 ($P4m2$): D_{2d}—$1a(s)$, $1b(i)$; C_{2v}—$\underline{2e}(s,i)$, $\underline{2f}(s,i)$, $\underline{2g}(s,i)$; C_2—$\underline{4h}(i)$; C_s—$\underline{\underline{4j}}(i)$, $\underline{\underline{4k}}(i)$; C_1—$\underline{\underline{\underline{8l}}}(i)$.

DG 32 ($Pnm2_1$): C_s—$\underline{\underline{2a}}(s,i)$; C_1—$\underline{\underline{\underline{4b}}}(i)$.

DG 24 ($Pmm2$): C_{2v}—$\underline{1a}(s,i)$, $\underline{1b}(s,i)$; C_s—$\underline{\underline{2e}}(s,i)$, $\underline{\underline{2f}}(s,i)$, $\underline{\underline{2g}}(i)$; C_1—$\underline{\underline{\underline{4i}}}(i)$.

DG 69 ($P3m1$): C_{3v}—$\underline{1a}(s,i)$, $\underline{1b}(s,i)$, $\underline{1c}(s,i)$; C_s—$\underline{\underline{3d}}(i)$; C_1—$\underline{\underline{\underline{6e}}}(i)$.

The band-state symmetries of a QW can be deduced from the band-state symmetries of a SL keeping, in the triperiodic 3D group of the SL, the Wyckoff positions of the corresponding diperiodic group of the QW. The k points to be taken from the corresponding 2D Brillouin zone (BZ) are the $k_z = 0$ cross section of the 3D BZ. When the barrier thickness in SL's goes to infinity, the k states of SL's transform into states of QW's with the same in-plane wave vector. The states of QW's with an in-plane wave vector equal to zero (Γ states) can thus be considered as the limit of Γ states in SL's. Since for any growth direction the QW point group coincides with the point group of the corresponding SL, the transitions between a bound state and a confined Γ state within the QW obey the same selection rules that transitions between a bound state and a Γ state do in SL's (Tables II–IV).

V. DISCUSSION

There are only a few papers devoted to experimental and theoretical studies of the impurity and defect states[4,10] in SL's. In these papers, the CD states in SL's are treated assuming that the site symmetry of substitutional impurities is the same as in parent tetrahedral materials, i.e., the T_d symmetry. Even more, in Ref. 4, where variational calculations were made for lowest donor states with a variety of SL parameters, the SL symmetry was not analyzed, the problem being solved within a continuous model. Such a state of art in the theory may lead to misinterpretations of experimental data.

Our approach for identification of CD's is based on their possible site symmetries in SL's and QW's (Tables I and VI and Secs. II and IV) and on the interpretation of the polarized optical spectra using the derived selection rules (Tables II–V). In addition, assuming that the types of CD's in heterostructures are in close correspondence with those in parent materials, we can use the results of investigations about dopants in the bulk materials (GaAs or III-V in general) as well as features of the growth technique. The main kind of simple CD in GaAs is antisite substitution of As with Ga in the case of the Ga-rich growth.[13] In the case of As-rich growth, which is usual for epitaxial-growth methods, the main kinds are the vacancy of Ga (V_{Ga}) and the $\mathrm{As}_{\mathrm{Ga}}$ antisite substitutions. Vacancies are mobile. They can thus migrate in the material, and be trapped by an antisite impurity to form complexes: $(V_{\mathrm{Ga}}, \mathrm{Ga}_{\mathrm{As}})$ and $(V_{\mathrm{As}}, \mathrm{As}_{\mathrm{Ga}})$. Though the energies of the latter complexes may be different, they are similar from the symmetry point of view when located at the same Ga and As atom positions. Presumably, such complexes act as nonradiative recombination centers in III-V materials.[14] Finally it has to be stressed that a specific feature may occur even in undoped GaAs/AlAs heterostructures: in addition to the vacancies and antisite substitutions taking place in pure III-V crystals, isovalent substitutions become possible when a Ga atom is replaced by an Al atom, or vice versa.

Finally, one can obtain additional information about optical transitions between extended and localized states in SL's and QW's by considering the splitting of CD states when lowering the symmetry from T_d in GaAs. Let us take as an example the anion-antisite defect $(\mathrm{Ga}_{\mathrm{As}})$. In GaAs this gives rise to a deep state with a_1 symmetry, and above it to a state with t_2 symmetry (see, e.g., Ref. 4). In SL's and QW's, the

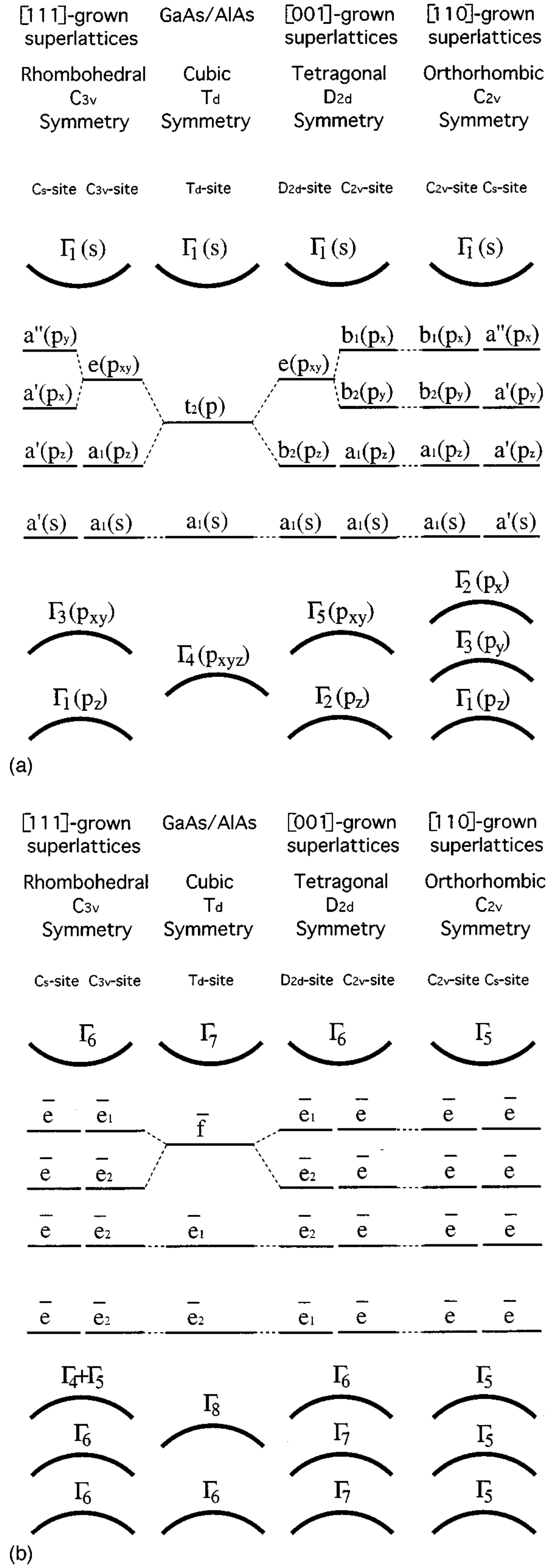

FIG. 3. Symmetry correspondence between the CD states in bulk GaAs(AlAs), and those localized at different sites in GaAs/AlAs SL's and QW's grown along different directions (a) neglecting spin-orbit interaction, and (b) with spin-orbit interaction included.

s-derived a_1 state corresponds to the a_1 state, whereas t_2 splits. Such a splitting takes place for any site. Figure 3(a) presents such transformations of states. The spin-orbit coupling additionally splits, and mixes various states [Fig. 3(b)]. The transformation of the Γ states, which are drawn in bold lines, is also shown.

Based on the procedure mentioned above, we can discuss, as an example, the experimental results given in Ref. 4. The authors observed,[4] in the $(GaAs)_5(AlAs)_5$ [001]-grown SL, a Ga-centered point-defect state with a_1 symmetry instead of the t_2 one they were expecting, since they assumed a T_d site symmetry for any substitutional impurity. Therefore, they assigned an interstitial character to the CD (Ga_i rather than Ga_{As}). However, as one can see from Table I, in [001]-grown SL's there are two types of As sites (of D_{2d} and C_{2v} symmetries). The former is absent in SL's with odd values of m and n, and the t_2 state splits into $a_1+b_1+b_2$. Thus the observed CD may be not an interstitial defect but a C_{2v} antisite one.

VI. CONCLUSION

The main results of the present paper can be formulated as follows.

(1) For $(GaAs)_m(AlAs)_n$ SL's grown along the [001], [110], and [111] directions, we have determined the site symmetries for various types of CD's: substitutional impurities, vacancies, interstitial impurities, and molecular CD's. It has been established that the distribution of the CD's over the Wyckoff positions depends not only on the growth direction but also on the number of monolayers constituting the SL unit cell. Moreover, each type of atom of the SL can be found at atomic positions with two different site symmetries in most of the [001]- and [110]-grown SL's.

(2) For CD's located at different sites in the SL's, we derived the selection rules for optical transitions between states of a CD and between CD states and Γ-band states, the spin-orbit interaction being taken into account. It has been shown how including this interaction modifies the localized states and optical transitions. An optical transition involving a CD can be allowed either completely or in certain polarizations, due to the appropriate symmetries of involved states, and/or due to spin-orbit interaction. When the transition is allowed only from the spin-orbit interaction, its oscillator strength is weaker. It is worth noting that the intensity of a line in the optical spectra also depends on the atomic arrangement over the Wyckoff positions. The larger the occupation number of a position in the primitive cell, the higher the intensity of a transition involving band (or localized) states induced by the atoms in this position.

(3) In general, we also showed a possibility of obtaining information about the sites of dopants in the lattice when analyzing the polarized optical spectra. Taking into account the energy and intensity of lines in the spectra, one can obtain information on the type of CD's which occupies the site.

(4) We presented the three-dimensional diperiodic space groups of QW's, and showed that QW's offer no difference from SL's either for possible site symmetries of various types of CD's or for optical selection rules involving them.

Summing up, the exact symmetries of various types of CD's in GaAs/AlAs QW'S and SL's were presented, along with selection rules for optical transitions involving them. The results we obtained are also valid for any pseudomorphic SL or QW made up of two binary compounds with the zinc-blende structures and identical anions or cations, such as in the GaN/AlN system.

ACKNOWLEDGMENTS

The authors acknowledge NATO Grant No. HTEC.CRG 960664, and thank Mairie de Paris for its support.

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