Electronic surface states and miniband structure of superlattices with multiple layers per period

E. H. El Boudouti
Département de Physique, Faculté des Sciences, Université de Oujda, Morocco

B. Djafari-Rouhani, A. Akjouj, and L. Dobrzynski
Laboratoire de Dynamique et Structure des Matériaux Moleculaires, Centre National de la Recherche Scientifique (URA 801), UFR de Physique, Université de Lille I, 59655 Villenueve d'Ascq Cedex, France

R. Kucharczyk* and M. Stęślicka
Institute of Experimental Physics, University of Wrocław, plac Maksa Borna 9, 50-204 Wrocław, Poland

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The electronic structure of a semi-infinite complex-basis superlattice (SL) with N layers per period is investigated, with emphasis placed on the effect of the SL surface (i.e., the SL/substrate interface). The bulk dispersion relation as well as the energy expression and existence condition for surface states are derived using the transfer-matrix method within an envelope-function approximation. Some common properties of a symmetric termination of the SL potential (i.e., when the substrate is identical to the last layer of the SL basis) are discussed and it is shown that—contrary to binary SL's—surface states can appear in complex-basis SL's also without perturbing the SL potential at the surface. These general results are illustrated by application to GaAs/$Al_xGa_{1-x}As$ SL's with four-layer (two-well and two-barrier) bases. [S0163-1829(97)01640-8]

I. INTRODUCTION

Recent advances in epitaxial crystal-growth techniques led to an experimental realization of the idea of polytype superlattices (SL's), initially proposed in Ref. 1. Consequently, in the last decade, semiconductor superlattices with the so-called *complex basis*, i.e., N layers per period ($N>2$), have been intensively studied both theoretically[2–9] and experimentally.[10–14] The motivation for such a study is based mainly on the following reasons. Polytype SL's provide more degrees of freedom when engineering the electronic structure as compared to typical, i.e., binary (two-layer period) SL's. In the latter, there are, in fact, three variables only, namely, the thicknesses of the wells and barriers and the barrier height. When additional layers are introduced in each SL period, more parameters are available, so an unusual electronic miniband structure can be obtained which is of a great value for modeling electrooptic devices with desired properties. To be more specific, a possibility of controlling the miniband and minigap widths independently offers several important applications including infrared photodetectors, effective-mass filtering, and tunning of the tunneling current.[6,7,11]

On the other hand, advanced growth techniques enabled experimentalists to create and study a prescribed *internal surface* (i.e., the SL/substrate interface) in a very controlled manner in binary SL's.[15–18] In particular, this resulted in the first observation[15] of a surface state in its pure form, i.e., as a single quantum state, in accordance with a classical paper by Tamm.[19,20] It has also been found[15–17,21–27] that the necessary condition for such a surface state to exist in a terminated binary SL is either the surface potential barrier (i.e., the substrate potential) to be sufficiently higher (lower) than the barriers inside SL or the outermost SL well to be sufficiently wider (narrower) than the interior ones.

Using SL's with a complex basis offers another opportunity for the surface-state occurrence. In our previous paper,[28] a particular case of such a SL, namely, the two-barrier basis SL, was investigated, and it was shown that—contrary to binary SL's—surface states can appear also without modifying the outermost SL period (the so-called *symmetric termination* of the SL potential).

To study this problem in a more comprehensive way, here we consider a terminated SL with N layers per period. The bulk dispersion relation as well as the energy expression and existence condition for surface states are derived, and some common properties of a symmetric termination of the SL potential are discussed. These general results are illustrated by application to GaAs/$Al_xGa_{1-x}As$ SL's with four-layer (two-well and two-barrier) bases.

II. MODEL OF *N*-LAYER BASIS SUPERLATTICE

The considered structure, as shown in Fig. 1, is a semi-infinite, periodic sequence of SL cells ($n=0,1,2,\ldots$) terminated by a semi-infinite homogeneous medium, representing the substrate. Each SL cell consists of N layers with the corresponding thicknesses d_j, potential heights V_j and effective masses m_j ($j=1,2,\ldots,N$); $D=d_1+d_2+\cdots+d_N$ stands for the SL period. The respective substrate parameters are denoted by V_s and m_s. A similar model has recently been applied to study the vibrational properties of a terminated complex-basis SL.[29]

III. GENERAL FORMALISM

Throughout the paper, the transfer-matrix method within an envelope-function approximation is used, as it seems to be most suitable for treating a general case of the N-layer basis SL. As a first step, the bulk dispersion relation is de-

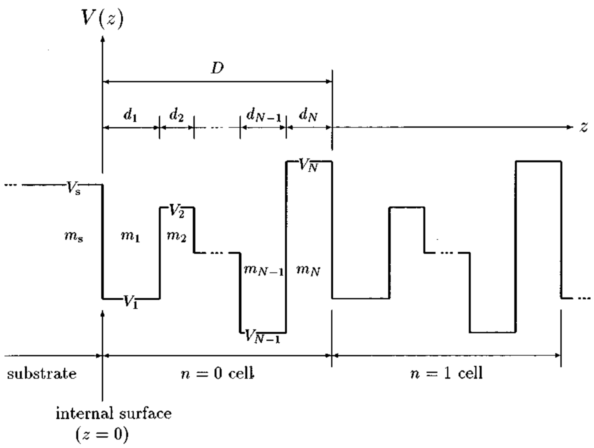

FIG. 1. Potential profile of a semi-infinite SL with N layers per period. For notation, see the text.

rived. For this purpose, we consider the SL as presented in Fig. 1, but consisting of an *infinite* sequence of cells. Next, the effect of an internal surface is taken into account in a *semi-infinite* SL, and the energy expression as well as existence condition for surface states are obtained for an arbitrary terminating medium.

A. Infinite superlattice

The wave function in the layer j of the cell n can be written as

$$\psi(n,j,z)=[A_j e^{-\alpha_j z}+B_j e^{\alpha_j z}]e^{iknD}, \tag{1}$$

where

$$\alpha_j=\frac{1}{\hbar}\sqrt{2m_j(V_j-E)};$$

E is the energy of an electron, k is the SL Bloch wave vector, and A_j and B_j are constants.

Applying the so-called Bastard's boundary conditions[30,31] to the wave function of the form of Eq. (1) at the interface between layers j and $j+1$ results in

$$\begin{pmatrix} e^{-(1/2)\,\alpha_j d_j} & e^{(1/2)\,\alpha_j d_j} \\ -F_j e^{-(1/2)\,\alpha_j d_j} & F_j e^{(1/2)\,\alpha_j d_j} \end{pmatrix}\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \begin{pmatrix} e^{(1/2)\,\alpha_{j+1} d_{j+1}} & e^{-(1/2)\,\alpha_{j+1} d_{j+1}} \\ -F_{j+1} e^{(1/2)\,\alpha_{j+1} d_{j+1}} & F_{j+1} e^{-(1/2)\,\alpha_{j+1} d_{j+1}} \end{pmatrix}\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix}, \tag{2}$$

which can formally be written, for any $j=1,2,\ldots,N$, as

$$H_j\begin{pmatrix} A_j \\ B_j \end{pmatrix}=K_{j+1}\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix}. \tag{3}$$

In Eq. (2),

$$F_j=\frac{\hbar^2}{2m_j}\alpha_j .$$

From Eq. (3) it follows that

$$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix}=S\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \tag{4}$$

where S is a transfer matrix given by

$$S=K_{N+1}^{-1}H_N K_N^{-1}H_{N-1}\ldots H_2 K_2^{-1}H_1 . \tag{5}$$

Since $K_{N+1}=K_1$ [cf. Eqs. (3) and (2), and Fig. 1], then

$$S=K_1^{-1}\Delta_N\Delta_{N-1}\ldots\Delta_2 H_1 , \tag{6}$$

with $\Delta_j=H_j K_j^{-1}$ having a simple form

$$\Delta_j=\begin{pmatrix} c_j & F_j^{-1}s_j \\ F_j s_j & c_j \end{pmatrix}, \quad j=1,2,\ldots,N, \tag{7}$$

where $c_j=\cosh(\alpha_j d_j)$ and $s_j=\sinh(\alpha_j d_j)$.

Combining the Bloch theorem

$$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix}=\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}e^{ikD} \tag{8}$$

with Eq. (4) leads to

$$(S-e^{ikD}I)\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}=0. \tag{9}$$

The requirement for nontrivial solutions of Eq. (9) reads

$$\det|S-e^{ikD}I|=0, \tag{10}$$

or, equivalently [cf. Eq. (6)],

$$\det|T_{1,\ldots,N}-e^{ikD}I|=0, \tag{11}$$

where

$$T_{1,\ldots,N}=\Delta_N\Delta_{N-1}\ldots\Delta_2\Delta_1 \tag{12}$$

has been introduced as a particularly useful form of the transfer matrix.

Thanks to a simplicity of Eqs. (12) and (7), the elements of matrix $T_{1,\ldots,N}$ can be given in a closed analytical form (see also Ref. 29), namely,

$$(T_{11})_{1,\ldots,N}=\sum_{\substack{\{j_1>j_2>\cdots>j_{N-2p}\} \\ \{j_{N-2p+1}>j_{N-2p+2}>\cdots>j_N\}}} c_{j_1}c_{j_2}\ldots c_{j_{N-2p}}s_{j_{N-2p+1}}s_{j_{N-2p+2}}\ldots s_{j_N}\frac{F_{j_N}}{F_{j_{N-1}}}\frac{F_{j_{N-2}}}{F_{j_{N-3}}}\cdots\frac{F_{j_{N-2p+2}}}{F_{j_{N-2p+1}}}, \tag{13a}$$

$$(T_{12})_{1,\ldots,N}=\sum_{\substack{\{j_1>j_2>\cdots>j_{N-2p-1}\} \\ \{j_{N-2p}>j_{N-2p+1}>\cdots>j_N\}}} c_{j_1}c_{j_2}\ldots c_{j_{N-2p-1}}s_{j_{N-2p}}s_{j_{N-2p+1}}\ldots s_{j_N}\frac{F_{j_{N-1}}}{F_{j_N}}\frac{F_{j_{N-3}}}{F_{j_{N-2}}}\cdots\frac{F_{j_{N-2p+1}}}{F_{j_{N-2p+2}}}\frac{1}{F_{j_{N-2p}}}, \tag{13b}$$

$$(T_{21})_{1,\ldots,N}=\sum_{\substack{\{j_1>j_2>\cdots>j_{N-2p-1}\}\\ \{j_{N-2p}>j_{N-2p+1}>\cdots>j_N\}}} c_{j_1}c_{j_2}\ldots c_{j_{N-2p-1}}s_{j_{N-2p}}s_{j_{N-2p+1}}\ldots s_{j_N}\frac{F_{j_N}}{F_{j_{N-1}}}\frac{F_{j_{N-2}}}{F_{j_{N-3}}}\cdots\frac{F_{j_{N-2p+2}}}{F_{j_{N-2p+1}}}F_{j_{N-2p}}, \tag{13c}$$

$$(T_{22})_{1,\ldots,N}=\sum_{\substack{\{j_1>j_2>\cdots>j_{N-2p}\}\\ \{j_{N-2p+1}>j_{N-2p+2}>\cdots>j_N\}}} c_{j_1}c_{j_2}\ldots c_{j_{N-2p}}s_{j_{N-2p+1}}s_{j_{N-2p+2}}\ldots s_{j_N}\frac{F_{j_{N-1}}}{F_{j_N}}\frac{F_{j_{N-3}}}{F_{j_{N-2}}}\cdots\frac{F_{j_{N-2p+1}}}{F_{j_{N-2p+2}}}. \tag{13d}$$

Each sum contains 2^{N-1} different terms and, e.g., the first term in summation in Eq. (13a) or (13d), corresponding to $p=0$, should be understood as $c_N c_{N-1}\ldots c_1$.

From Eq. (11) one can obtain, using the unitary property of matrix $T_{1,\ldots,N}$,

$$\cos(kD)=\tfrac{1}{2}[(T_{11})_{1,\ldots,N}+(T_{22})_{1,\ldots,N}]. \tag{14}$$

Equation (14) stands for the bulk dispersion relation $E=E(k)$ for a complex-basis SL with N layers per period. Taking advantage of Eqs. (13), the right-hand side of Eq. (14) can be explicited in a closed form (cf. Refs. 5 and 13), which, however, is too complicated for further analytical handling in the case of a general multilayer basis (for particular bases see Sec. V), so Eq. (14) has to be solved numerically.[32] In particular, the miniband edges can be found by equating the right-hand side of Eq. (14) to ± 1.

For any solution of Eq. (14), the corresponding wave function can also be obtained. Indeed, Eq. (9) gives the ratio A_1/B_1, which—assuming A_1 to be a normalization constant—yields B_1, while all the remaining coefficients A_j and B_j $(j=2,3,\ldots,N)$ can be calculated from Eq. (2).

B. Semi-infinite superlattice

The wave function of a surface state can still be written, inside the SL ($z>0$ in Fig. 1), in the form of Eq. (1). The SL Bloch wave vector k, however, is now complex ($k=i\mu+l\pi/D$, $\mu>0$, $l=0,\pm1,\pm2,\ldots$) to ensure a decaying character of $\psi(n,j,z)$ toward the SL. Obviously, the wave vector satisfies the bulk dispersion relation given by Eq. (14).

In the substrate region ($z<0$ in Fig. 1), the corresponding wave function is

$$\psi_s(z)=B_s e^{\alpha_s z}, \tag{15}$$

where

$$\alpha_s=\frac{1}{\hbar}\sqrt{2m_s(V_s-E)}.$$

Bastard's boundary conditions applied to the SL and substrate wave functions at the internal surface ($z=0$ in Fig. 1) give

$$\begin{pmatrix}0 & 1\\ 0 & F_s\end{pmatrix}\begin{pmatrix}0\\ B_s\end{pmatrix}=\begin{pmatrix}e^{(1/2)\,\alpha_1 d_1} & e^{-(1/2)\,\alpha_1 d_1}\\ -F_1 e^{(1/2)\,\alpha_1 d_1} & F_1 e^{-(1/2)\,\alpha_1 d_1}\end{pmatrix}\begin{pmatrix}A_1\\ B_1\end{pmatrix}, \tag{16}$$

with

$$F_s=\frac{\hbar^2}{2m_s}\alpha_s .$$

Eliminating B_s from Eq. (16) yields the ratio of A_1 to B_1:

$$\frac{A_1}{B_1}=\frac{F_1-F_s}{F_1+F_s}\,e^{-\alpha_1 d_1}. \tag{17}$$

This ratio, however, is also determined by Eq. (9), viz.

$$\frac{A_1}{B_1}=\frac{S_{12}}{e^{ikD}-S_{11}}. \tag{18}$$

Equating the right-hand sides of Eqs. (17) and (18) leads to the dispersion relation for surface states:

$$e^{ikD}=S_{11}+S_{12}\frac{F_1+F_s}{F_1-F_s}\,e^{\alpha_1 d_1}. \tag{19}$$

A more symmetric form of the surface-state-energy expression can be obtained by combining e^{ikD} and e^{-ikD} [cf. Eq. (19)], and taking into account the bulk dispersion relation [cf. Eq. (14)]. It reads

$$S_{11}-S_{22}+S_{12}\frac{F_1+F_s}{F_1-F_s}\,e^{\alpha_1 d_1}-S_{21}\frac{F_1-F_s}{F_1+F_s}\,e^{-\alpha_1 d_1}=0. \tag{20}$$

Replacing the elements of the matrix S by those of the matrix $T_{1,\ldots,N}$ [cf. Eqs. (6) and (12)] results in the following energy expression for surface states of an arbitrarily terminated N-layer basis SL:

$$F_s^2(T_{12})_{1,\ldots,N}+F_s[(T_{11})_{1,\ldots,N}-(T_{22})_{1,\ldots,N}]-(T_{21})_{1,\ldots,N}=0. \tag{21}$$

Since for a surface state k is complex, the inequality

$$|e^{ikD}|<1 \tag{22}$$

must hold to ensure a decaying character of the surface-state wave function toward the SL. Taking into account Eq. (19) and remembering that k satisfies Eq. (14) this leads to the following necessary condition for a surface state to exist:

$$|(T_{22})_{1,\ldots,N}-F_s(T_{12})_{1,\ldots,N}|>1. \tag{23}$$

In other words, the validity of Eq. (23) should be checked for any solution of Eq. (21) to assure that it corresponds to the true surface-state energy.

Using the explicit expressions for $(T_{ij})_{1,\ldots,N}$, $i,j=1,2$ [cf. Eqs. (13)], both Eqs. (21) and (23) can be written in a closed form. In the case of a general complex basis (for particular bases, see Sec. V), however, they can be hardly handled analytically and numerical calculations have to be performed.

The surface-state wave function can also be constructed. Assuming again A_1 to be a normalization constant, Eq. (16) gives B_s and B_1, while Eq. (2) yields all the remaining coefficients A_j and B_j $(j=2,3,\ldots,N)$.

IV. SYMMETRIC TERMINATION OF SUPERLATTICE POTENTIAL

The term *symmetric termination* of the SL potential is coined here to describe the case of the substrate being identical to the last layer of the SL basis. It means $m_s=m_N$ and $V_s=V_N$ (cf. Fig. 1) and, consequently, $\alpha_s=\alpha_N$ and $F_s=F_N$. Then Eqs. (21) and (23) become

$$F_N^2(T_{12})_{1,\ldots,N}+F_N[(T_{11})_{1,\ldots,N}-(T_{22})_{1,\ldots,N}]-(T_{21})_{1,\ldots,N}=0 \tag{24}$$

and

$$|(T_{22})_{1,\ldots,N}-F_N(T_{12})_{1,\ldots,N}|>1, \tag{25}$$

respectively.

From Eq. (12) it follows that

$$T_{1,\ldots,N}=\Delta_N T_{1,\ldots,N-1}, \tag{26}$$

which, taking into account the explicit form of matrix Δ_N [cf. Eq. (7)], leads to the following set of equations relating the matrix elements of $T_{1,\ldots,N}$ to those of $T_{1,\ldots,N-1}$:

$$(T_{11})_{1,\ldots,N}=c_N(T_{11})_{1,\ldots,N-1}+s_NF_N^{-1}(T_{21})_{1,\ldots,N-1}, \tag{27a}$$

$$(T_{12})_{1,\ldots,N}=c_N(T_{12})_{1,\ldots,N-1}+s_NF_N^{-1}(T_{22})_{1,\ldots,N-1}, \tag{27b}$$

$$(T_{21})_{1,\ldots,N}=s_NF_N(T_{11})_{1,\ldots,N-1}+c_N(T_{21})_{1,\ldots,N-1}, \tag{27c}$$

$$(T_{22})_{1,\ldots,N}=s_NF_N(T_{12})_{1,\ldots,N-1}+c_N(T_{22})_{1,\ldots,N-1}. \tag{27d}$$

Inserting Eqs. (27) into Eqs. (24) and (25) yields

$$(c_N-s_N)\{F_N^2(T_{12})_{1,\ldots,N-1}+F_N[(T_{11})_{1,\ldots,N-1}-(T_{22})_{1,\ldots,N-1}]-(T_{21})_{1,\ldots,N-1}\}=0 \tag{28}$$

and

$$(c_N-s_N)|(T_{22})_{1,\ldots,N-1}-F_N(T_{12})_{1,\ldots,N-1}|>1, \tag{29}$$

respectively. Since

$$(c_N-s_N)=e^{-\alpha_N d_N}\neq 0,$$

the surface-state-energy expression for the N-layer basis SL terminated in a symmetric way [Eq. (28)] becomes exactly the same as the energy expression for surface states of the $(N-1)$-layer basis SL terminated by the substrate with V_N and m_N [cf. Eq. (21)]. Although the energy expression [Eq. (28)] does not now depend on the thickness d_N of the last layer forming the SL basis, one should have in mind that the solutions of Eq. (28) correspond to surface-state energies provided the existence condition [Eq. (29)] is satisfied. The latter, however, does not reproduce the surface-state existence condition for the $(N-1)$-layer basis SL terminated by the substrate with V_N and m_N [cf. Eq. (23)], as it can be rewritten as

$$|(T_{22})_{1,\ldots,N-1}-F_N(T_{12})_{1,\ldots,N-1}|>e^{\alpha_N d_N}, \tag{30}$$

indicating a strong dependence on d_N. In particular, for d_N large enough, Eq. (30) is never satisfied, so surface states cannot appear.

Generally, however, we can conclude that—contrary to binary SL's—surface-state occurrence is possible in multilayer basis SL's terminated in a symmetric way, i.e., without perturbing the SL potential at the surface. Moreover, as long as the surface state exists, its energy is independent of the thickness of the last layer forming the SL basis whenever this layer is identical to the substrate.

This striking property can be related to the specific shape of the surface-state wave function in such a case. Indeed, following the prescription given in Sec. III B with $\alpha_s=\alpha_N$ and $F_s=F_N$ one arrives at

$$A_N=\{F_N^2(T_{12})_{1,\ldots,N-1}+F_N[(T_{11})_{1,\ldots,N-1}-(T_{22})_{1,\ldots,N-1}]-(T_{21})_{1,\ldots,N-1}\}B_s \tag{31a}$$

and

$$B_N=\{F_N^2(T_{12})_{1,\ldots,N-1}+F_N[(T_{11})_{1,\ldots,N-1}+(T_{22})_{1,\ldots,N-1}]+(T_{21})_{1,\ldots,N-1}\}e^{\alpha_N d_N}B_s. \tag{31b}$$

However, since for a surface state Eq. (28) is satisfied, $A_N=0$. Thus the surface-state wave function in the layer N of any cell n takes the single exponential form[33]

$$\psi(n,N,z)=B_Ne^{\alpha_N z}e^{iknD}. \tag{32}$$

As a consequence, the logarithmic derivative of the wave function inside the layer N is position independent, and, therefore, the thickness d_N does not enter the surface-state-energy expression [Eq. (28)].

V. APPLICATION TO FOUR-LAYER BASES

The general formalism presented in Secs. III and IV for a semi-infinite SL with an N-layer basis is applied here to the most commonly investigated polytype SL, namely, the *biperiodic* SL.[3,4,6–9] The period of such a SL consists, in general, of four different layers: two arbitrary wells alternating with two arbitrary barriers. To reduce the number of variable parameters, however, we restrict our considerations to the simplest biperiodic bases, namely, the *two-barrier basis* (two identical wells coupled via barriers of the same height and different width) and the *two-well basis* (two wells of a different thickness coupled via identical barriers).

In both cases, the formulas for the bulk dispersion relation as well as the energy expression and existence condition for surface states can be written explicitly in quite a concise manner. This not only allows to confirm general properties, but makes a further analytical consideration possible.

Selected numerical results are also presented to illustrate analytical findings. All the computations have been per-

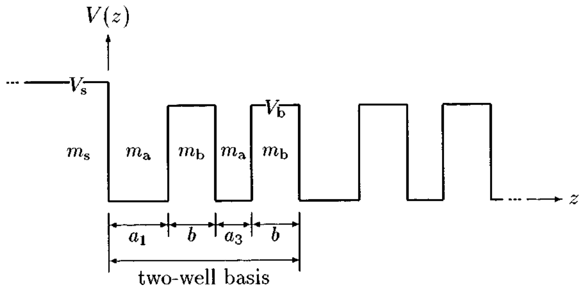

FIG. 2. Potential profile of a semi-infinite two-well basis SL. For notation, see the text.

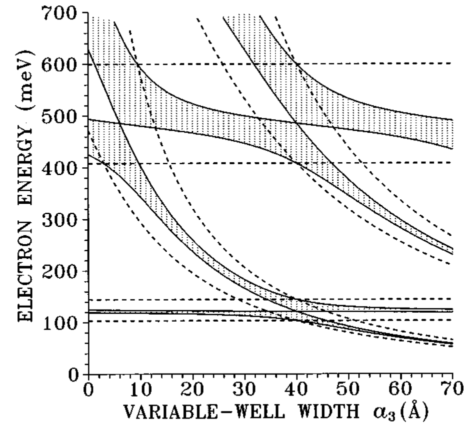

FIG. 3. Electronic bulk band structure of a two-well basis GaAs/$Al_{0.5}Ga_{0.5}As$ SL with $a_1 = 40$ Å, $b = 20$ Å, and variable a_3 (shaded areas). For comparison, miniband edges of the component binary SL's with the well (a_1)/barrier (b) and well (a_3)/barrier (b) bases are also presented (dashed lines).

formed for SL's made out of GaAs and $Al_xGa_{1-x}As$, as this choice enables one to realize and manipulate a wide range of potential profiles.[34]

A. Two-well basis

Potential profile of a terminated two-well basis SL is sketched in Fig. 2. To make the parameters describing well and barrier regions easily distiguishable, the notation has been somewhat changed with respect to that used for a general complex basis (cf. Fig. 2 vs Fig. 1): m_a, m_b, and m_s are now the effective-mass values in the well layers, barrier layers, and the substrate, respectively, V_b and V_s denote the height of the SL and substrate potential barriers, correspondingly (zero of the potential is deliberately chosen at the well bottom), while a_1, a_3, and b stand for the respective layer thicknesses. For convenience we shall refer to particular SL layers as the well (a_1), well (a_3), and barrier (b) [the well (a_1) is always assumed to be in contact with substrate].

In this notation, the bulk dispersion relation for a two-well basis SL reads [cf. Eqs. (14) and (13)]

$$\cos(kD) = 2B_{a_1+b}(E)B_{a_3+b}(E) - c_{a_3-a_1}, \tag{33}$$

where $c_{a_3-a_1} = \cosh[\alpha_a(a_3 - a_1)]$ (please have in mind that $V_a = 0$, so α_a is pure imaginary). In Eq. (33), $B_{a_1+b}(E)$ and $B_{a_3+b}(E)$ stand for the right-hand side of the bulk dispersion relation of a binary SL with the well (a_1)/barrier (b) and well (a_3)/barrier (b) basis, respectively, viz.

$$\cos(k_{a_1+b}D_{a_1+b}) = c_{a_1}c_b + \frac{1}{2}\left(\frac{F_a}{F_b} + \frac{F_b}{F_a}\right)s_{a_1}s_b \equiv B_{a_1+b}(E) \tag{34a}$$

and

$$\cos(k_{a_3+b}D_{a_3+b}) = c_{a_3}c_b + \frac{1}{2}\left(\frac{F_a}{F_b} + \frac{F_b}{F_a}\right)s_{a_3}s_b \equiv B_{a_3+b}(E), \tag{34b}$$

where $c_{a_1} = \cosh(\alpha_a a_1)$, $c_{a_3} = \cosh(\alpha_a a_3)$, $c_b = \cosh(\alpha_b b)$, $s_{a_1} = \sinh(\alpha_a a_1)$, $s_{a_3} = \sinh(\alpha_a a_3)$, and $s_b = \sinh(\alpha_b b)$, $D_{a_1+b} = a_1 + b$ and $D_{a_3+b} = a_3 + b$ denote the periods, while k_{a_1+b} and k_{a_3+b} are the Bloch wave vectors of the corresponding two-layer basis SL's.

The bulk band structure of four-layer basis SL's has been already studied[3,4,6–9] and it has been concluded, basing on numerical results, that the electronic structure of a biperiodic SL can be, to large extent, considered as a superposition of minibands of the constituent binary SL's. Our result for a two-well basis SL is in agreement with previous reports, moreover, the explicit form of Eq. (33) seems to be particularly helpful for analytical handling.

For example, if the wells are of equal width, i.e., $a_1 = a_3$, Eq. (33) reduces to

$$\cos(kD) = 2[B_{a_1+b}(E)]^2 - 1, \tag{35}$$

indicating that the minibands of the four-layer basis SL coincide then with those of the corresponding two-layer basis SL. Indeed, when $B_{a_1+b}(E)$ varies from 1 (-1) to -1 (1), the right-hand side of Eq. (35) varies from 1 to -1 and back to 1, with no minigap opening at $k = \pi/D$, i.e., at the Brillouin-zone boundary of the four-layer basis SL. For identical wells, however, $k = \pi/D$ is equivalent to $k_{a_1+b} = \pi/(2D_{a_1+b})$ being in the midst of the Brillouin zone of the two-layer basis SL, as the doubled SL periodicity is then artificial and so is the doubled Brillouin-zone folding.

Furthermore, whenever $B_{a_1+b}(E) = 0$ or $B_{a_3+b}(E) = 0$ is satisfied, Eq. (33) yields $|\cos(kD)| \leqslant 1$, indicating that an energy corresponding to the middle of the miniband of either component two-layer basis SL also lies within the miniband of the two-well basis SL. On the other hand, if both $|B_{a_1+b}(E)| > 1$ and $|B_{a_3+b}(E)| > 1$ hold, Eq. (33) gives $|\cos(kD)| > 1$, so any energy from the common section of minigaps of the two binary SL's falls also into the minigap of the biperiodic SL. In other words, all the minibands of the two-well basis SL are contained within the superimposed minibands of the constituent SL's.

This is demonstrated in Fig. 3, where the calculated miniband edges of a two-well basis GaAs/$Al_{0.5}Ga_{0.5}As$ SL with $a_1 = 40$ Å and $b = 20$ Å, and variable a_3 are plotted (solid lines delimiting shaded areas) and compared to those of both component binary SL's (dashed lines). It is clear that the overall electronic structure results from mixing of minibands originating from SL's with a constant-width well (horizontal bands) and a variable-width well (falling bands). Whenever there is an overlap of minibands of two constituent SL's (the

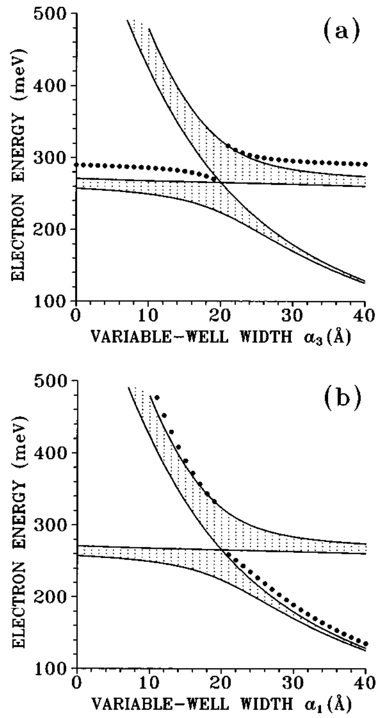

FIG. 4. Surface electronic structure of a semi-infinite two-well basis GaAs/$Al_{0.6}Ga_{0.4}As$ SL with (a) $a_1 = b = 20$ Å and variable a_3 and (b) $a_3 = b = 20$ Å and variable a_1, terminated by the AlAs substrate. Shaded areas correspond to the minibands, while full dots indicate the position of surface states.

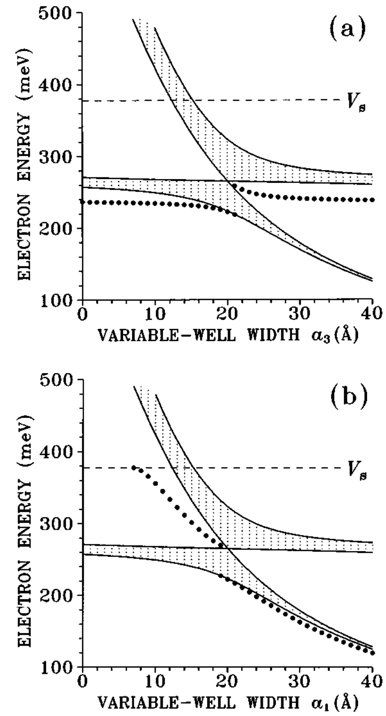

FIG. 5. The same as in Fig. 4, but for the $Al_{0.4}Ga_{0.6}As$ substrate. The dashed line indicates the surface potential barrier height V_s.

so-called band alignment), a band splitting is observed in the resulting structure. Away from the band-crossing points, the bandwidth is significantly reduced, since the nonsymmetrical well acts as a barrier for nonaligned minibands.

Terminating the SL potential, as has been generally shown in Secs. III and IV, opens a possibility for surface states to appear inside the minigaps. For a two-well basis SL, the surface-state-energy expression and the corresponding existence condition become [cf. Eqs. (21), (23), and (13)]

$$2B_{a_3+b}(E)\left[\left(\frac{F_s}{F_a}-\frac{F_a}{F_s}\right)s_{a_1}c_b+\left(\frac{F_s}{F_b}-\frac{F_b}{F_s}\right)c_{a_1}s_b + \left(\frac{F_a}{F_b}-\frac{F_b}{F_a}\right)s_{a_1}s_b\right]+\left(\frac{F_s}{F_a}-\frac{F_a}{F_s}\right)s_{a_3-a_1}=0 \tag{36}$$

and

$$\left|\frac{F_s}{F_a}\left[\left(\frac{F_b}{F_a}s_{a_3}c_b+c_{a_3}s_b\right)s_{a_1}s_b+s_{a_3+a_1}c_b^2\right] + \frac{F_s}{F_b}\left[\left(\frac{F_a}{F_b}s_{a_3}s_b+c_{a_3}c_b\right)c_{a_1}s_b+c_{a_3+a_1}c_b s_b\right] - 2B_{a_3+b}(E)\left(\frac{F_b}{F_a}s_{a_1}s_b+c_{a_1}c_b\right)+c_{a_3-a_1}\right|>1, \tag{37}$$

respectively, where $c_{a_3+a_1}=\cosh[\alpha_a(a_3+a_1)]$, $s_{a_3+a_1}=\sinh[\alpha_a(a_3+a_1)]$, and $s_{a_3-a_1}=\sinh[\alpha_a(a_3-a_1)]$.

As one can see, the formulas obtained for an arbitrary terminating medium are rather complicated. However, for the substrate made out of the same material as the SL barriers ($m_s = m_b$ and $V_s = V_b$ in Fig. 2), Eqs. (36) and (37) can be substantially simplified by putting $\alpha_s = \alpha_b$ and $F_s = F_b$. This yields

$$2B_{a_3+b}(E)s_{a_1}e^{-\alpha_b b}+s_{a_3-a_1}=0 \tag{38}$$

and

$$\left|\frac{F_b}{F_a}[2B_{a_3+b}(E)s_{a_1}e^{-\alpha_b b}+s_{a_3-a_1}] - 2B_{a_3+b}(E)c_{a_1}e^{-\alpha_b b}+c_{a_3-a_1}\right|>1 \tag{39}$$

for the energy expression and existence condition for surface states of a two-well basis SL terminated in a symmetric way. From combined Eqs. (39) and (38), a much simpler form of the necessary condition for surface states to occur immediately follows, viz.

$$|s_{a_3}|>|s_{a_1}|. \tag{40}$$

Essential properties of the surface electronic structure of a semi-infinite two-well basis SL are illustrated in Figs. 4–6. Computations have been performed for GaAs/$Al_{0.6}Ga_{0.4}As$ SL's with $a_1 = b = 20$ Å and variable a_3, as well as with $a_3 = b = 20$ Å and variable a_1, to compare the effect of the SL termination on a constant- or variable-width well. Various surface conditions have been taken into account by considering different substrates, namely, AlAs (to get $V_s > V_b$), $Al_{0.4}Ga_{0.6}As$ (to get $V_s < V_b$), and $Al_{0.6}Ga_{0.4}As$ (to get $V_s = V_b$, i.e., symmetric termination of the SL potential).

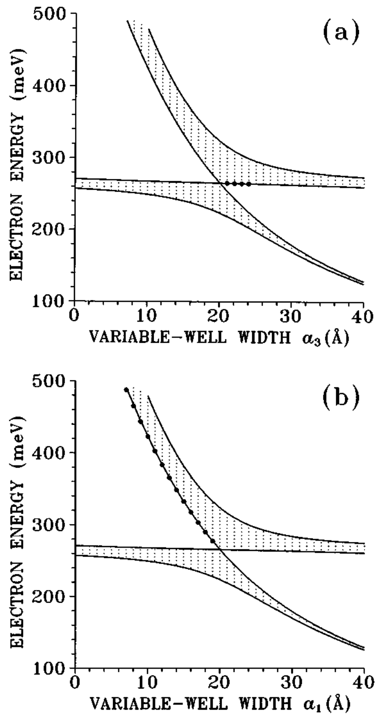

FIG. 6. The same as in Fig. 4, but for the $Al_{0.6}Ga_{0.4}As$ substrate (symmetric termination of the SL potential).

As it can be seen in Figs. 4 and 5, the surface potential barrier sufficiently high or low, with respect to the SL barriers, causes a surface state to appear above or below the corresponding miniband, respectively. A similar behavior has been found before for terminated binary SL's.[15–17,21–27] For a two-well basis SL, however, surface states detach only from minibands originating from the eigenstates of the outermost well. Indeed, surface-state-energy curves follow the horizontal or falling bands depending on whether a_3 or a_1 is variable [cf. Figs. 4(a) and 5(a) vs Figs. 4(b) and 5(b)]. Moreover, inspection of the corresponding wave functions (not shown) indicates that all the surface states are localized mostly in the well being in contact with substrate.

Figure 6 demonstrates the possibility of surface-state occurrence for a symmetric termination of the SL potential when using a two-well complex basis, in contrast to the typical two-layer basis of a single well and barrier. However, for a wide range of SL parameters, i.e., acceptable layer thicknesses and barrier heights, it is virtually impossible to obtain a surface state well separated from the miniband edges. As a consequence, the existing surface states are rather poorly localized, and their wave functions exhibit Bloch-like character with almost no damping toward the SL. In practice, such surface states should not actually modify the bulk electronic properties of two-well basis SL's.

B. Two-barrier basis

A semi-infinite two-barrier basis SL is schematically shown in Fig. 7. Characteristic parameters are the same as for a two-well basis SL (cf. Sec. V A and Fig. 2) except for a, b_2, and b_4 denoting now the well and two different barrier thicknesses, respectively [the barrier (b_2) is always assumed to be closer to the SL surface].

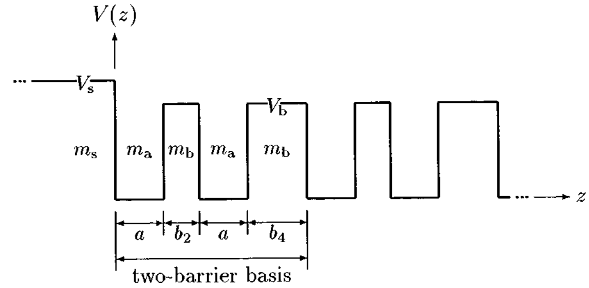

FIG. 7. Potential profile of a semi-infinite two-barrier basis SL. For notation, see the text.

The bulk dispersion relation for a two-barrier basis SL can also be written in a concise form [cf. Eqs. (14) and (13)], namely,

$$\cos(kD)=2B_{a+b_2}(E)B_{a+b_4}(E)-c_{b_4-b_2}, \tag{41}$$

where $c_{b_4-b_2}=\cosh[\alpha_b(b_4-b_2)]$, while $B_{a+b_2}(E)$ and $B_{a+b_4}(E)$ are the right-hand side of the bulk dispersion relation of a binary SL with the well (a)/barrier (b_2) and well (a)/barrier (b_4) basis, correspondingly [cf. Eqs. (34) and (33)].

Analysis of Eq. (41), similar to that of Eq. (33), leads to the conlcusion that for identical barriers ($b_2=b_4$) the miniband structure of a four-layer basis SL again reproduces that of the respective two-layer basis SL. If $b_2\neq b_4$, however, the minigap can always be found in the electronic structure of a two-barrier basis SL around energies corresponding to the middle of miniband of either component binary SL. Indeed, whenever $B_{a+b_2}(E)=0$ or $B_{a+b_4}(E)=0$ holds, so the energy corresponds to $k_{a+b_2}=\pi/(2D_{a+b_2})$ or $k_{a+b_4}=\pi/(2D_{a+b_4})$, being in the midst of the Brillouin zone of the respective two-layer basis SL; Eq. (41) yields $\cos(kD)<-1$, indicating clearly the minigap opening at $k=\pi/D$, i.e., at the Brillouin-zone boundary of the four-layer basis SL. Consequently, each degenerated miniband of the constituent binary SL's splits into two minibands of the biperiodic SL due to a perturbation introduced by a different second barrier in the SL basis.

This is confirmed by the miniband structure calculations performed for a two-barrier basis $GaAs/Al_{0.5}Ga_{0.5}As$ SL with $a=60$ Å, $b_2=15$ Å, and variable b_4. The corresponding numerical results are presented in Fig. 8.

The energy expression for surface states in a two-barrier basis SL terminated by an arbitrary medium reads [cf. Eqs. (21) and (13)]

$$2B_{a+b_2}(E)\left[\left(\frac{F_s}{F_a}-\frac{F_a}{F_s}\right)s_ac_{b_4}+\left(\frac{F_s}{F_b}-\frac{F_b}{F_s}\right)c_as_{b_4}+\left(\frac{F_a}{F_b}-\frac{F_b}{F_a}\right)s_as_{b_4}\right]+\left(\frac{F_s}{F_b}-\frac{F_b}{F_s}\right)s_{b_2-b_4}=0, \tag{42}$$

together with the existence condition [cf. Eqs. (23) and (13)]

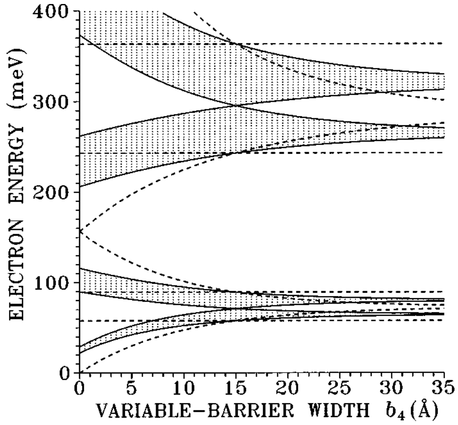

FIG. 8. Electronic bulk band structure of a two-barrier basis GaAs/$Al_{0.5}Ga_{0.5}As$ SL with $a=60$ Å, $b_2=15$ Å, and variable b_4 (shaded areas). For comparison, miniband edges of the component binary SL's with the well (a)/barrier (b_2) and well (a)/barrier (b_4) bases are also presented (dashed lines).

$$\left|\frac{F_s}{F_a}\left[\left(\frac{F_b}{F_a}s_a s_{b_2}+c_a c_{b_2}\right)s_a c_{b_4}+c_{b_2+b_4}c_a s_a\right] + \frac{F_s}{F_b}\left[\left(\frac{F_a}{F_b}c_a s_{b_2}+s_a c_{b_2}\right)s_a s_{b_4}+s_{b_2+b_4}c_a^2\right] - 2B_{a+b_2}(E)\left(\frac{F_b}{F_a}s_a s_{b_4}+c_a c_{b_4}\right)+c_{b_2-b_4}\right|>1. \tag{43}$$

Since, however, we are interested mostly in the effect of SL termination by the substrate identical to the SL barriers ($m_s=m_b$ and $V_s=V_b$ in Fig. 7), we simplify Eqs. (42) and (43) by replacing α_s and F_s with α_b and F_b, respectively. They become

$$B_{a+b_2}(E)=0 \tag{44}$$

and

$$\left|2B_{a+b_2}(E)\left(\frac{F_b}{F_a}s_a-c_a\right)+e^{\alpha_b b_2}\right|e^{-\alpha_b b_4}>1, \tag{45}$$

correspondingly. Furthermore, we substitute Eq. (44) into Eq. (45) and arrive at

$$e^{\alpha_b(b_2-b_4)}>1$$

or

$$b_2>b_4 \tag{46}$$

as the necessary condition for a surface state to exist.

Consequently, surface states can appear in a two-barrier basis SL terminated in a symmetric way, provided the barrier lying closer to the surface is wider than the other one. This indicates—in accordance with the general conclusions of Sec. IV—a critical dependence of the surface-state occurrence on the thickness of the barrier (b_4).

Conversely, as follows from Eq. (44), the surface-state energy does not depend on b_4, confirming again the findings of Sec. IV. Moreover, it lies in the range corresponding to the middle of miniband of a constituent binary SL. It has been pointed out, however, that if Eq. (46) holds (which is the necessary condition for a surface state to occur), a minigap opens around the energy satisfying Eq. (44). Hence, we really deal with a true surface state.

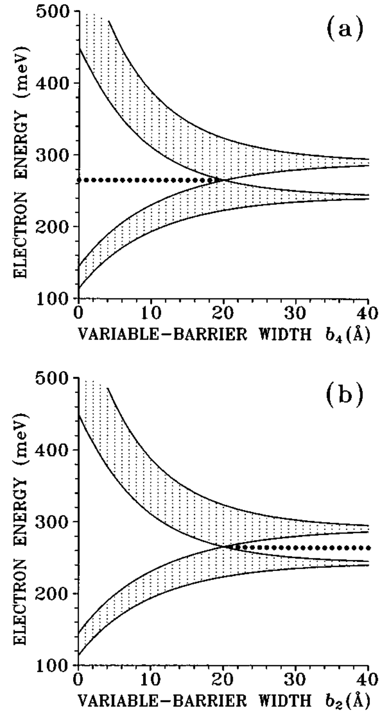

FIG. 9. Surface electronic structure of a semi-infinite two-barrier basis GaAs/$Al_{0.6}Ga_{0.4}As$ SL with (a) $a=b_2=20$ Å and variable b_4 and (b) $a=b_4=20$ Å and variable b_2, terminated by the $Al_{0.6}Ga_{0.4}As$ substrate (symmetric termination of the SL potential). Shaded areas correspond to the minibands, while full dots indicate the position of surface states.

This specific surface-state behavior is illustrated in Fig. 9 for GaAs/$Al_{0.6}Ga_{0.4}As$ SL's with $a=b_2=20$ Å and variable b_4, as well as with $a=b_4=20$ Å and variable b_2, being in contact with the $Al_{0.6}Ga_{0.4}As$ substrate. As it can be seen, the opportunity of a well-defined surface state to exist even for the terminating medium identical to the SL barriers is unambiguously realized in a two-barrier basis SL. In contrast to the previously studied two-well basis SL (cf. Fig. 6), surface states resulting from a symmetric termination of the SL potential are now clearly separated from the miniband edges and, thus, are strongly confined to the SL surface. Since the miniband splitting takes place exactly at $b_2=b_4$, the surface state—to keep Eq. (46) satisfied—appears within just one of the minigaps opening at the band crossing point.

As has been shown before for terminated binary SL's,[35,36] the energy-level occurrence within a minigap, corresponding to a state localized at the SL end, could—under certain conditions—lead to an effective removal of the forbidden energy gap. Therefore, the existence of surface states should be taken into account when device applications of SL's are considered.

For completeness, the results of surface electronic structure computations for two-barrier basis GaAs/$Al_{0.6}Ga_{0.4}As$ SL's with other substrates, namely, $Al_{0.8}Ga_{0.2}As$ (to get $V_s>V_b$) and $Al_{0.5}Ga_{0.5}As$ (to get $V_s<V_b$), are shown in Figs. 10 and 11, respectively. The effect of a different sur-

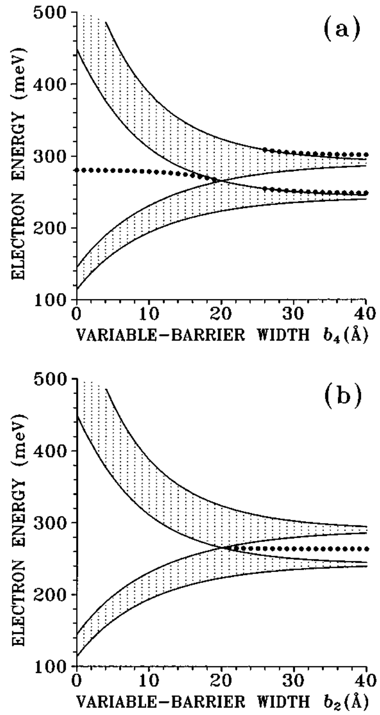

FIG. 10. The same as in Fig. 9, but for the $Al_{0.8}Ga_{0.2}As$ substrate.

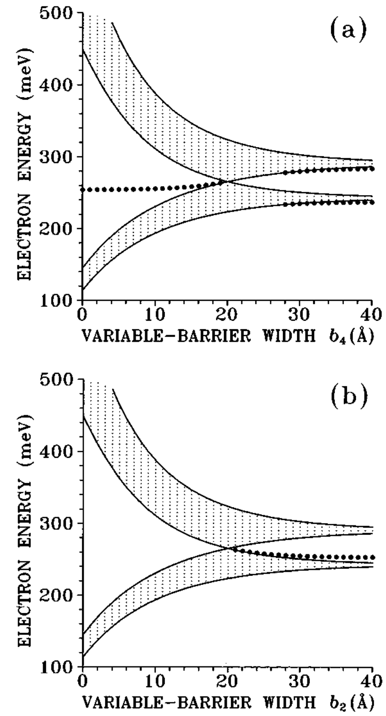

FIG. 11. The same as in Fig. 9, but for the $Al_{0.5}Ga_{0.5}As$ substrate.

facepotential barrier is similar to that observed for two-well basis SL's and agrees with previous findings for terminated binary SL's.[22,24–27] Analysis of the surface-state wave functions (not shown) indicates that again all the surface states are localized mostly in the outermost well.

VI. SUMMARY

In this work, the electronic structure of a semi-infinite complex-basis SL with N layers per period has been investigated. Using the transfer-matrix method within an envelope-function approximation, the bulk dispersion relation has been derived for a general multilayer basis. The effect of the SL surface (i.e., the SL/substrate interface) has been studied, and the energy expression as well as existence condition for surface states have been obtained for an arbitrary terminating medium.

Special attention has been paid to the case of a symmetric termination of the SL potential, i.e., when the substrate is identical to the last layer of the SL basis ($m_s = m_N$ and $V_s = V_N$ in Fig. 1). It has been shown that—in contrast to typical, i.e., two-layer basis SL's—surface states can appear in complex-basis SL's also without modifying the outermost SL period. In such a case, the surface-state energy does not depend on the thickness of the last layer forming the SL basis; however, the corresponding existence condition critically does.

The general formalism has been applied to terminated GaAs/$Al_xGa_{1-x}As$ SL's with a two-well basis (two wells of a different thickness coupled via identical barriers) and a two-barrier basis (two identical wells coupled via barriers of the same height and different width). In both cases, the formulas for the bulk dispersion relation as well as the energy expression and existence condition for surface states have been explicitly written in a very concise manner. This enabled us to conclude essential properties of the electronic structure, basing on analytical considerations and use the numerical results mostly for illustration.

The performed calculations indicate a possibility of well-defined surface states to occur in complex-basis SL's. As was pointed out, their existence is of importance when device applications of SL's are considered.

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*Author to whom correspondence should be addressed.

[1] L. Esaki, L. L. Chang, and E. E. Mendez, Jpn. J. Appl. Phys. **20**, L529 (1981).

[2] G. Bastard, Phys. Rev. B **25**, 7584 (1982).

[3] H. X. Jiang, Phys. Rev. B **33**, 5851 (1986).

[4] H. X. Jiang and J. Y. Lin, Am. J. Phys. **55**, 462 (1987).

[5] B. Djafari-Rouhani and L. Dobrzynski, Solid State Commun. **62**, 609 (1987).

[6] P. Yuh and K. L. Wang, Phys. Rev. B **38**, 13 307 (1988).

[7] P. Vasilopoulos, F. M. Peeters, and D. Aitelhabti, Phys. Rev. B **41**, 10 021 (1990).

[8] G. Ihm, S. K. Noh, J. I. Lee, S. J. Lee, and T. W. Kim, Superlattices Microstruct. **12**, 155 (1992).

[9] J. Shi and S. Pan, Phys. Rev. B **48**, 8136 (1993).

[10] M. Nakayama, K. Kubota, S. Chika, H. Kato, and N. Sano, Solid State Commun. **58**, 475 (1986).

[11] K. K. Choi, B. F. Levine, C. G. Bethea, J. Walker, and R. J. Malik, Phys. Rev. Lett. **59**, 2459 (1987).
[12] H. Schneider, K. Kawashima, and K. Fujiwara, Phys. Rev. B **44**, 5943 (1991).
[13] D. J. Lockwood, R. L. S. Devine, A. Rodriguez, J. Mendialdua, B. Djafari-Rouhani, and L. Dobrzynski, Phys. Rev. B **47**, 13 553 (1993).
[14] F. Agulló-Rueda, H. T. Grahn, and K. Ploog, J. Appl. Phys. **79**, 8106 (1996).
[15] H. Ohno, E. E. Mendez, J. A. Brum, J. M. Hong, F. Agulló-Rueda, L. L. Chang, and L. Esaki, Phys. Rev. Lett. **64**, 2555 (1990).
[16] F. Agulló-Rueda, E. E. Mendez, H. Ohno, and J. M. Hong, Phys. Rev. B **42**, 1470 (1990).
[17] H. Ohno, E. E. Mendez, A. Alexandrou, and J. M. Hong, Surf. Sci. **267**, 161 (1992).
[18] T. Miller and T.-C. Chiang, Phys. Rev. Lett. **68**, 3339 (1992).
[19] I. E. Tamm, Phys. Z. Sowjetunion **1**, 733 (1932).
[20] S. G. Davison and M. Stęślicka, *Basic Theory of Surface States* (Clarendon, Oxford, 1992).
[21] M. Stęślicka, R. Kucharczyk, and M. L. Glasser, Phys. Rev. B **42**, 1458 (1990).
[22] W. L. Bloss, Phys. Rev. B **44**, 8035 (1991).
[23] R. Kucharczyk and M. Stęślicka, Solid State Commun. **81**, 557 (1992).
[24] P. Masri, Surf. Sci. Rep. **19**, 1 (1993).
[25] E.-H. El Boudouti, R. Kucharczyk, and M. Stęślicka, Czech. J. Phys. **43**, 899 (1993).
[26] M. Stęślicka, R. Kucharczyk, E.-H. El Boudouti, B. Djafari-Rouhani, M. L. Bah, A. Akjouj, and L. Dobrzynski, Vacuum **46**, 459 (1995).
[27] M. Stęślicka, Prog. Surf. Sci. **50**, 65 (1995).
[28] R. Kucharczyk, M. Stęślicka, E.-H. El Boudouti, A. Akjouj, L. Dobrzynski, and B. Djafari-Rouhani, Czech. J. Phys. **47**, 421 (1997).
[29] E.-H. El Boudouti, B. Djafari-Rouhani, A. Akjouj, and L. Dobrzynski, Phys. Rev. B **54**, 14 728 (1996).
[30] D. J. BenDaniel and C. B. Duke, Phys. Rev. **152**, 683 (1966).
[31] G. Bastard, Phys. Rev. B **24**, 5693 (1981).
[32] Numerical solutions to Eq. (14) can be obtained in a straightforward way by fixing E at every step and finding k, rather than vice versa, as this does not require any particular root-finding routine, and enables one to avoid the problem of spurious solutions.
[33] It is worth noticing that the wave function of the form of Eq. (32) can be directly obtained from that given by Eq. (15) by applying the Bloch theorem—this is justified, as for the substrate identical to the last layer forming the SL basis, the SL potential may be regarded as periodic up to the distance d_N inside the substrate.
[34] The potential barrier height of $Al_xGa_{1-x}As$ is determined by $V=944x$ meV, while the corresponding effective mass is given by $m=(0.067+0.083x)m_{el}$, m_{el} being the free-electron mass (after Ref. 15).
[35] R. Kucharczyk and M. Stęślicka, Solid State Commun. **84**, 727 (1992).
[36] M. Stęślicka and R. Kucharczyk, Vacuum **45**, 211 (1994).