Surface states in superlattices

Maria Stęślicka and Robert Kucharczyk
Institute of Experimental Physics, ulica Cybulskiego 36, PL-50-205 Wrocław, Poland

M. L. Glasser
Department of Mathematics and Computer Science, Clarkson University, Potsdam, New York 13676
(Received 29 September 1989; revised manuscript received 8 March 1990)

A terminated Kronig-Penney-like model is proposed for studying electronic surface states in compositional (potential-modulation) and in effective-mass (mass-modulation) superlattices. The existence of surface states in the minigaps of both types of superlattices is shown explicitly and their properties are discussed.

Semiconductor superlattices (SL) have been extensively investigated experimentally in recent years.[1] Considerable efforts have also been made to determine the electronic structure of these new materials using the envelope-function approach, pseudopotential methods and tight-binding approximation.[2] In a series of papers,[3-5] it has been shown that a classical Kronig-Penney analysis can serve as a useful approximation for calculating the electronic level structure of a semiconductor SL. This model shows that a conduction band of a SL consists of the electronic minibands alternating with minigaps with the bandwidths and effective masses in good agreement with experiment.[1]

However, a SL is composed of a few layers and thus the surface effects must be included in more realistic calculations. In particular, the possibility of the surface electronic structure in the minigaps (MG) of a thin periodic SL was studied using the tight-binding envelope approximation[6] and two-band model.[2] The obtained results suggest that, as expected, surface states can appear in MG. However, important physical parameters, such as the thickness and effective mass of particular layers, do not appear explicitly in the above mentioned approaches. Thus, the obtained results seem to have rather limited applicability.

The aim of the present paper is to propose a Kronig-Penney-like model appropriate for a terminated compositional SL (e.g., vacuum/GaAs/$Al_xGa_{1-x}As$/GaAs/$\cdots$) and mass-modulation SL (e.g., vacuum/$In_{0.69}Ga_{0.31}As$/InP/$In_{0.69}Ga_{0.31}As$/$\cdots$). By using the direct matching procedure we calculate analytically the energy and localization properties of surface states. Then, the corresponding expressions are solved numerically.

To obtain the conduction-band electronic structure of a semi-infinite compositional SL we assume a potential profile as shown in Fig. 1, i.e., consisting of alternating well and barrier layers of thicknesses a and b and effective masses m_1 and m_2, respectively. The potential V describes the differences in the conduction-band edges while the zero energy fits the GaAs conduction-band edge. The SL is terminated at the well region (GaAs) by the step potential $U \geq V$ representing the vacuum with the electron mass $m=1$ (in Hartree atomic units, used in this paper).

Using the direct matching procedure with Bastard's[7] boundary conditions at $z=a$ (Fig. 1) and Bloch requirement we can obtain the SL wave function for the first well layer ($0<z<a$) in the form

$$\Psi_{SL}(z)=A[\sin(kz)+\lambda\cos(kz)], \quad E<V \tag{1}$$

with A being a normalization constant and

$$\lambda=\frac{\sin(k_1a)+K\sinh(k_2b)\exp(ikd)}{\cosh(k_2b)\exp(ikd)-\cos(k_1a)} . \tag{2}$$

In Eqs. (1) and (2)

$$K=k_1m_2/k_2m_1 , \tag{3}$$

$k_1=(2m_1E)^{1/2}$, $k_2=(2m|E-V|)^{1/2}$, $d=a+b$ is a period of the SL, k is the wave number of an electron in the SL, and E is the energy of an electron. Here, we are interested only in localized electronic states lying inside MG. For the nth MG, k is complex and has the following form:

$$k=i\mu+n\pi/d, \quad \mu>0, \quad n=0,1,2,\ldots . \tag{4}$$

Inserting (4) into (1) shows that now the wave function decreases along the positive z axis by a factor of

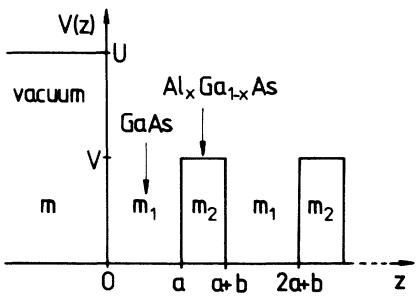

FIG. 1. Potential profile of a compositional superlattice. For notation see the text.

$\exp(-\mu d)$ and, thus, can be used to study localized surface states.

In the vacuum region ($z<0$), the wave function has the form

$$\Psi_V(z)=F\exp(k_3 z)\ , \tag{5}$$

where $k_3=[2(U-E)]^{1/2}$, F being a constant.

Using (4) and applying Bastard's boundary conditions to Eqs. (1) and (5) at $z=0$, i.e.,

$$\Psi_{SL}(0)=\Psi_V(0),\ m_1^{-1}\Psi'_{SL}(0)=\Psi'_V(0) \tag{6}$$

yields

$$(-1)^n\exp(-\mu d)=\frac{\sin(k_1 a)+G\cos(k_1 a)}{G\cosh(k_1 b)-K\sinh(k_2 b)}\equiv S(E)\ , \tag{7}$$

where

$$G=k_1/k_3 m_1\ . \tag{8}$$

On the other hand, the dependence $E(k)$ is given by the familiar, Kronig-Penney-type, expression.[3] For k complex [Eq. (4)], it has the form

$$(-1)^n\cosh\mu d=\cos k_1 a\cosh k_2 b + \tfrac{1}{2}(K^{-1}-K)\sin k_1 a\sinh k_2 b\equiv B(E)\ . \tag{9}$$

Eliminating μ from (7) and (9) gives the following energy equation for surface states in the nth MG:

$$S(E)-B(E)\pm[B^2(E)-1]^{1/2}=0\ , \tag{10}$$

where $+$ and $-$ correspond to n even and n odd, respectively.

The solutions of (10) give the energy of surface states as a function of the effective masses m_1 and m_2; layer thicknesses a and b; the barrier height V and the vacuum level U. Obviously m_2 and V depend on the crystal composition x.

The localization properties of the superlattice surface states (SSS) are examined with the help of the relative probability density function defined as[8]

$$P(z)=|\Psi(z)|^2/|\Psi(0)|^2\ . \tag{11}$$

All the above expressions have been derived for $E<V$. For $V<E<U$, a simple transformation $k_2\rightarrow ik_2$ should be made.

Equations (9)–(11) have been solved numerically for both the compositional and effective-mass SL. As an example of a terminated compositional SL we consider the case of the vacuum/GaAs/$Al_xGa_{1-x}As$/GaAs/$\cdots$ system (cf. Fig. 1). The electron effective mass in the GaAs wells, m_1, is taken to be 0.067 (in atomic units) while the effective mass in $Al_xGa_{1-x}As$ barriers, m_2, has the form (cf. Refs. 3 and 5)

$$m_2=m_1+0.083x\ .$$

The conduction band discontinuity or barrier height $V=V(x)$ is assumed to be[9]

$$V(x)=0.6\,\Delta E_\Gamma(x)\ ,$$

where $\Delta E_\Gamma(x)$ is the band-gap difference at the Γ minima between GaAs and $Al_xGa_{1-x}As$, and[10]

$$\Delta E_\Gamma(x)=\begin{cases}1.247x, & x<0.45\\ 1.247x+1.147(x-0.45)^2, & x>0.45\ .\end{cases}$$

It should be mentioned that the other conduction-band minimia in the momentum space, Γ–X or Γ–L, have not been considered in this paper. However, it was pointed out[4,11] that the electron coupling probability from Γ (X) to X (Γ) states is poor when compared with Γ-Γ states. For the value of U, the electron affinity of the outermost superlattices layer is taken, which for GaAs equals to 4.07 eV.[4]

Solving (9) and (10) leads to the energy spectrum of the terminated GaAs/$Al_xGa_{1-x}As$ SL consisting of minibands alternating with minigaps. The first and second MG are shown in Fig. 2, where shaded areas correspond to the miniband regions. The most interesting result is the appearance of the electronic levels inside each of the MG. Their wave functions exhibit decaying character inside the SL and in the direction of the vacuum [Figs. 3(a) and 3(b)]. Consequently, these levels can be recognized as superlattice surface states (SSS). The exponential decay factor R, being the ratio of the maxima of $P(z)$ in two adjacent SL cells, can serve as a measure of localization properties of the corresponding SSS. It should be added that the number of maxima of $P(z)$ in each cell always coincides with the MG number [cf. Figs. 3(a) and 3(b)], as in the well-known Tamm model.[8]

In the low-lying MG, there always exists one SSS (cf. Fig. 2). However, for the fourth and higher MG, two SSS can be observed. When the SSS energy comes closer to the miniband edge, its localization becomes weaker (i.e., R increases), in agreement with the results of Ref. 2. We also note that for small x and, in particular, for higher

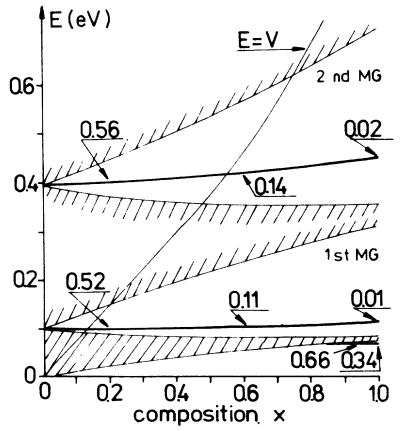

FIG. 2. Energy spectrum of the terminated GaAs/$Al_xGa_{1-x}As$ superlattice with the layer thicknesses $a=60$ Å and $b=15$ Å. Hatched areas correspond to the energy minibands, thick curves represent the energy of surface states, and underlined numbers denote the values of the localization factor R.

MG, R is close to 1, thus the corresponding SSS are Bloch-like. For larger values of x, the SSS eigenfunctions change and become highly localized near the "surface" ($z=0$ in Fig. 1). Similar behavior was reported in Ref. 6.

In the lowest ($n=0$) MG, the SSS detaches from the lower miniband edge at $x \gtrsim 0.85$ and its $P(z)$ exhibits one maximum in a cell, i.e., the same character as the SSS in the first MG. Since the lowest miniband is usually occupied for typical doping densities, the low-energy SSS should also be occupied and, thus, might be essential in various electronic processes.

Increasing (decreasing) U shifts the energies of the lowest minigap surface state towards (outwards) the band edge, and, as a consequence, worsens (improves) its localization. Therefore, for U larger (smaller) this SSS detaches from the band edge at larger (smaller) values of x, e.g., for $U \simeq 4.6$ eV the SSS occurs in the MG only for $x \simeq 1.0$ while for $U > 4.6$ eV there is no SSS in the lowest MG. The SSS in the first and second MG are almost unsensitive to the changes of the vacuum level. Increase (decrease) of U affects the localization of the SSS in such a way that $P(z)$ maxima are moved outwards (towards) the surface and the peaks are more (less) pronounced with respect to $P(z=0)$.

Recently, Sasaki[4] has proposed a new type of SL, where the effective mass of electrons is changed periodically and the conduction-band edge is aligned as to eliminate the potential discontinuities between the respective SL layers. Our model (Fig. 1) represents a terminated effective-mass superlattice (EMSL) when $V=0$. Following Sasaki's analysis for an infinite EMSL, we assume that

$$a/b=(m_2/m_1)^{1/2} \text{ or } k_1 a = k_2 b \ . \tag{12}$$

For numerical computations the case of the vacuum/$In_{0.69}Ga_{0.31}As$/InP/$In_{0.69}Ga_{0.31}As$/$\cdots$ system is taken with $m_1=0.034$ and $m_2=0.073$, respectively. Thus, according to (12), $a/b=1.47$. Now, $U \simeq 4.4$ eV.[4]

The numerical solution to Eqs. (9) and (10) with $V=0$ and Eq. 12 gives the energy spectrum of the EMSL consisting of minibands and minigaps. Inside the MG, the electronic states appear and are identified as the SSS because their $P(z)$ behave in a similar way as that shown in Fig. 3(a). The variation of the first MG (which for EMSL is the lowest one), with respect to the EMSL layer thickness is presented in Fig. 4. The new result, compared to Ref. 4, is the existence of SSS. One of them is always located at the midgap position and thus is characterized by the same value of the localization factor ($R=0.47$) and this does not depend on energy. The second SSS emerges from the lowest miniband at $a \gtrsim 35$ Å with $P(z)$ having also one maximum in the cell [cf. Fig. 3(a)]. However, since it lies close to the miniband edge its localization is much poorer and, in fact, for $a \simeq 40$ Å it exhibits a Bloch-like character. For larger values of a, the lower SSS becomes well localized (Fig. 4). The "midgap" state is almost unsensitive to the changes of U, while the second SSS moves towards higher (lower) energies when U is increased (decreased). However, these shifts are less than 10^{-3} eV even for $\Delta U = \pm 1$ eV. The SSS wave functions depend on U as in the case of the compositional superlattice.

To our best knowledge, the SSS in EMSL have not been previously studied. On the other hand, it has re-

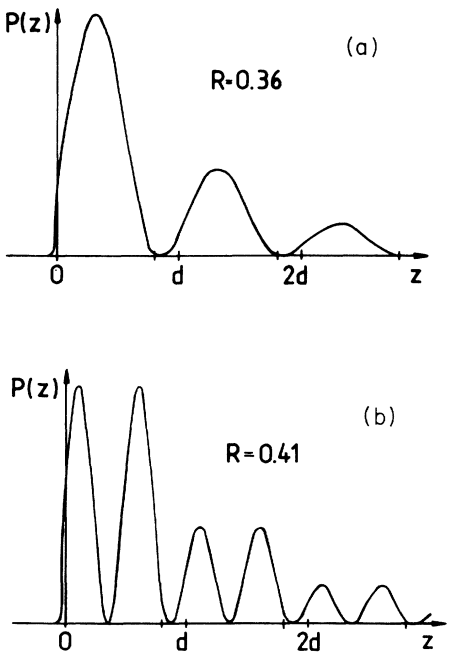

FIG. 3. Relative probability density function $P(z)$ for the surface states in (a) the first minigap and (b) the second minigap.

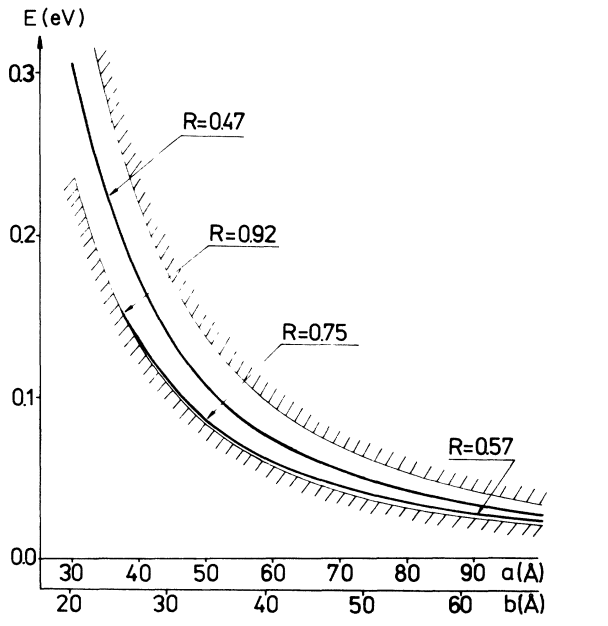

FIG. 4. Variation of the energy of the surface states lying inside the first minigap of the terminated $In_{0.69}Ga_{0.31}As$/InP effective-mass superlattice. Hatched areas correspond to the miniband regions.

cently been found that such SL exhibit a new type of negative resistance and a current density of 2 orders of magnitude greater than that of a compositional SL.[12] Thus, the surface states can play an important role in many phenomena occurring in the EMSL.

The presented model can easily be extended to include the heavy-hole and light-hole energy bands, to investigate the energy spectrum of finite SL such as, for example, $Al_xGa_{1-x}As/AlAs/GaAs/AlAs/\cdots/AlAs/Al_xGa_{1-x}As$, and to study the effect of the application of an electric field perpendicular to the layers. Such calculations are now in progress.

[1]L. Esaki, IEEE J. Quantum Electron. **QE-22**, 1611 (1986), and references therein.

[2]P. Masri, L. Dobrzynski, B. Djafari-Rouhani, and I. O. A Idiodi, Surf. Sci. **166**, 301 (1986), and references therein.

[3]V. Milanovic and D. Tjapkin, Phys. Status Solidi B **110**, 687 (1982).

[4]A. Sasaki, Phys. Rev. B **30**, 7016 (1984); Surf. Sci. **174**, 624 (1986).

[5]H.-S. Cho and P. L. Prucnal, Phys. Rev. B **36**, 3237 (1987).

[6]J. Zhang and S. E. Ulloa, Phys. Rev. B **38**, 2063 (1988).

[7]G. Bastard, Phys. Rev. B **24**, 5693 (1981).

[8]A. J. Thakkar and M. Stęślicka, Surf. Sci. **74**, 168 (1978).

[9]R. C. Miller, D. A. Kleinmann, and A. C. Gossard, Phys. Rev. B **29**, 7085 (1984).

[10]B. A. Vojak, W. D. Laidig, N. Holonyak, Jr., and M. D. Camras, J. Appl. Phys. **52**, 621 (1981).

[11]G. C. Osbourn, J. Appl. Phys. **53**, 1586 (1982).

[12]A. Aishima and Y. Fukushima, J. Appl. Phys. **61**, 249 (1987).