Calculation of electronic surface states in superlattices via graph formulations

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We propose a graph method for the analysis of electronic surface states in a complex basis superlattice terminated by surface with a multilayer clad. Using topology theory, we frame an energy equation for calculating the surface modes based on a graph model. Compared to the traditional methods, the present method does not have the problem of numerical instability for finding out the surface states of the superlattices. The other advantage is that the localized states are directly solved by the present method without spurious solutions, which usually exist in the solutions obtained by traditional methods. Numerical examples show removal of the spurious solutions by traditional methods may cause numerically instable and incorrect results.

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Semiconductor superlattices have been extensively researched and applied to microelectronics in recent years. Much attention has been paid to the characteristics of electron motion for the disturbed periodic superlattices, including terminated or defect structures [1–13]. Determination of the existence and properties of the localized electron states in semi-infinite superlattices can help fundamental physics examine the effect of the surface and defect on semi-infinite and finite superlattices [2–13]. For the terminated binary superlattices, the energy equation for surface states has been framed in analytical form [3,4]. The eigenenergy of each localized state can be determined according to the expression. Recently, polytype superlattices, composed of multiple layers in each cell, have received great interest in applications of high performance semiconductors [14,15]. For superlattices with a complex basis, various numerical methods have been applied to solve the localized states [16–19]. Of those methods, the transfer matrix method [2–4,19], is one of the most popular methods since it is easy to draw up the energy equation even for a great number of layers in the basis. However, the transfer matrix method suffers from numerical instability during calculation. Various schemes have been proposed to avoid the numerical instability problem but the analysis works will be more complex. Moreover, in traditional methods, the eigenvalues solved by the energy equation of the terminated superlattice usually include not only the actual roots but also the spurious ones. It is tedious to find out the spurious solutions from all of the solved roots using the condition of eigenfunction decay.

Graph theory [20,21] has been used to solve linear equations and analyze networks for a long time, but it is inconvenient for most of the applications. To our knowledge, the graph theory has not been applied on the analysis of electronic surface states of superlattices. In this study, we propose an eigenenergy equation for the surface states of the terminated superlattices based on the graph theory. Moreover, the eigenenergies for the surface states solved by the present equation include only actual roots without spurious ones.

A semi-infinite superlattice with N layers a cell and terminated at the left as shown in Fig. 1 is considered. We first study the behavior of electron motion in the part of the clad structure. The potential barrier heights, effective mass values, and thicknesses for layer j of the clad structure are $U_{c,j}$, $m^*_{c,j}$, and $d_{c,j}$, respectively. Using envelope-function approximation, the motion of an electron in the vicinity of the conduction band bottom for layer j of the clad can be expressed by a wave function $\psi(c,j,z)=a_{c,j}e^{ik_{c,j}(z-z_{c,j-1})}+b_{c,j}e^{-ik_{c,j}(z-z_{c,j-1})}$, where $k_{c,j}=\hbar^{-1}[2m^*_{c,j}(E-U_{c,j})]^{1/2}$. Here we define $\psi(c,j,z_{c,j})$ and $(m^*_e/k_e m^*_{c,j})\psi'(c,j,z_{c,j})$ as $\psi_{c,j}$ and $\theta_{c,j}$, respectively, in which $k_e=\hbar^{-1}(2m^*_e E_e)^{1/2}$, m^*_e is the electron mass, and E_e is a reference energy that is arbitrarily set as 1 eV. By the reference energy, these wave functions and their slope at the boundary of layer j can be expressed by dimensionless relations as

$$\begin{Bmatrix} \psi_{c,j} \\ \theta_{c,j-1} \end{Bmatrix} = \begin{bmatrix} f_j & h_j \\ g_j & f_j \end{bmatrix} \begin{Bmatrix} \psi_{c,j-1} \\ \theta_{c,j} \end{Bmatrix}, \tag{1}$$

where f_j, g_j, and h_j are equal to $\sec k_{c,j}d_{c,j}$, $\beta_j \tan k_{c,j}d_{c,j}$, and $\beta_j^{-1} \tan k_{c,j}d_{c,j}$, respectively, and $\beta_j=k_{c,j}m^*_e/(k_e m^*_{c,j})$. The relations given in Eq. (1) can be represented by a two-way graph model as shown in Fig. 2. According to Bastard's boundary conditions, $\psi_{c,j}$ and $\theta_{c,j}$ are continued at the intersection of layer j and $j+1$. Thus the graph models for all of the layers in the clad can be connected and expressed by

$$\begin{Bmatrix} \psi_{c,N_c} \\ \theta_{c,0} \end{Bmatrix} = \begin{bmatrix} f_c & h_c \\ g_c & f_c \end{bmatrix} \begin{Bmatrix} \psi_{c,0} \\ \theta_{c,N_c} \end{Bmatrix}, \tag{2}$$

where f_c, g_c, and h_c can be calculated by the graph theory [20,21] based on the graph model for the clad

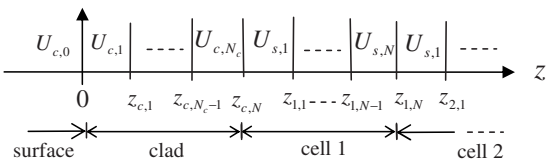

FIG. 1. Potential profile of an N-layer basis superlattice terminated by the surface and an N_c-layer clad barrier.

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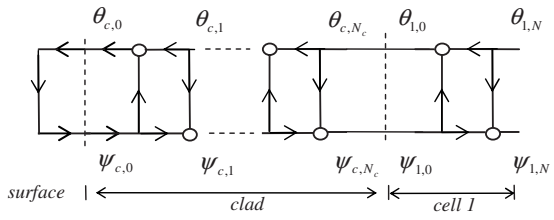

FIG. 2. Graph model for the analysis of the terminated superlattice with the surface and a multilayer clad barrier.

as $(\Pi_{j=1}^{N_c} f_j)/S^{1,N_c}$, $(\Sigma_{p=1}^{N_c} g_p S^{p,N_c} \Pi_{j=1}^{p-1} f_j^2)/S^{1,N_c}$, and $(\Sigma_{p=1}^{N_c} h_p S^{1,p} \Pi_{j=p+1}^{N_c} f_j^2)/S^{1,N_c}$, in which $S^{p,q}$ is the determinant of a part of the graph model for the structure from layers p to q given by $S^{p,q} = \Sigma_{v=0}^{q-p} \Sigma_{i_{2v}=p+v}^{q} \Sigma_{i_{2v-1}=p+v-1}^{i_{2v}-1} \cdots \Sigma_{i_2=p+1}^{i_3} \Sigma_{i_1=p}^{i_2-1} \Pi_{u=1}^{v} (-G_{i_{2u-1},i_{2u}})$ and $G_{p,q}$ is $h_p g_q \Pi_{j=p}^{q} f_j^2$.

For the surface barrier, it is assumed there is no rightward wave coming from the left-hand side (LHS). If the wave function in the surface barrier is expressed by $\psi(c,0,z) = b_{c,0} e^{-ik_{c,0}z}$, we have $\theta_{c,0} = -ik_{c,0} m_e^* \psi_{c,0}/(k_e m_{c,0}^*)$. According to Eq. (2), the relation between ψ_{c,N_c} and θ_{c,N_c} determined by the terminated structure is $\psi_{c,N_c} = \theta_{c,N_c}[h_c - k_e m_{c,0}^* f_c^2/(ik_{c,0} m_e^* + k_e m_{c,0}^* g_c)]$.

For the periodic superlattice connected to the right-hand side (RHS) of the surface cell, we can represent the relations between $\psi_{1,0}$ and $\theta_{1,0}$ as $\theta_{1,0} = R_s \psi_{1,0}$. From the connection of the terminated structure and the superlattice, we have $\psi_{c,N_c} = \psi_{1,0}$ and $\theta_{c,N_c} = \theta_{1,0}$. Thus, the eigenvalue equation for the surface mode is

$$1 - R_s \left(h_c - \frac{k_e m_{c,0}^* f_c^2}{ik_{c,0} m_e^* + k_e m_{c,0}^* g_c} \right) = 0. \tag{3}$$

We next look at the electron motion in the periodic superlattices, which is connected to the right end of the clad structure as described in Fig. 1. In each cell of the superlattice, the potential barrier heights, effective mass values, and thicknesses for layer j of each cell are $U_{s,j}$, $m_{s,j}^*$, and $d_{s,j}$, respectively. For the periodic superlattices, the wave functions in layer j of cell n can be expressed by the same forms as Eqs. (1) and (2), respectively, with c replaced by n. In the same way, we represent the wave functions at the boundary of cell 1 by the forms

$$\begin{Bmatrix} \psi_{1,N} \\ \theta_{1,0} \end{Bmatrix} = \begin{bmatrix} f_s & h_s \\ g_s & f_s \end{bmatrix} \begin{Bmatrix} \psi_{1,0} \\ \theta_{1,N} \end{Bmatrix}, \tag{4}$$

where $\psi_{1,j}$ and $\theta_{1,j}$ are defined by $\psi(1,j,z_{1,j})$ and $m_e^* \psi'(1,j,z_{1,j})/(k_e m_{s,j}^*)$, respectively.

According to Floquet's theorem, the envelope functions in a periodic system must obey the Bloch waves. For cell 1 of the periodical superlattice, we can write the relations of the envelope functions at the right and left ends of the cell as $\theta_{1,N} = \theta_{1,0} \exp(iKL)$ and $\psi_{1,0} = \psi_{1,N} \exp(-iKL)$. By substituting the relation of $\theta_{1,N}$ and $\theta_{1,0}$ into Eq. (4) and using the relation of $\theta_{1,0} = R_s \psi_{1,0}$, we have

$$R_s = \frac{g_s}{1 - f_s e^{iKL}}. \tag{5}$$

Substituting $\theta_{1,N} = \theta_{1,0} \exp(iKL)$ and $\psi_{1,0} = \psi_{1,N} \exp(-iKL)$ into Eq. (4), we have $f_s e^{2iKL} - \chi_s e^{iKL} + f_s = 0$, where $\chi_s = 1 - g_s h_s + f_s^2$. Thus, the solution of the Bloch phase is given by $e^{iKL} = [\chi_s \pm (\chi_s^2 - 4f_s^2)^{1/2}]/(2f_s)$. Since the eigenfunction in the superlattice decays with the increase of the distance from the surface, the absolute value of the exponential function should be less than one, $|e^{iKL}| < 1$. Thus, only one of the $\pm$ signs in the solution is reasonable. If the sign $+$ is chosen for $\chi_s \geq 0$ and $-$ for $\chi_s < 0$, the absolute value of e^{iKL} will be less than 1. So, the reasonable e^{iKL} is changed by a sign-number function α and rewritten in the form

$$e^{iKL} = \frac{\chi_s - \alpha(\chi_s^2 - 4f_s^2)^{1/2}}{2f_s}, \tag{6}$$

where α is equal to 1 if the value of $(1 + g_s h_s - f_s^2)$ is greater than or equal to zero, and -1 if it is less than zero. Equation (3) with Eqs. (5) and (6) is the major equation of this paper.

For the numerical performance of the present theory, a four-layer superlattice made of $Al_xGa_{1-x}As$ and terminated by a surface of AlAs is first examined. The Al concentration for each layer is $x_1 = x_3 = 0$ and $x_2 = x_4 = 0.5$. The width of each layer is $d_1 = 4$ nm and $d_2 = d_3 = d_4 = 2$ nm. If we define the left-hand side of Eq. (3) as the characteristic function J_c, the roots of $J_c = 0$ are matching to eigenvalues for the surface modes and shown in Fig. 3. Also, two transfer matrix methods proposed by Stęślicka *et al.* [2] and Huang *et al.* [19], denoted by TMM-S and TMM-H respectively, are examined to compare. The energy equations to solve the surface modes in both transfer matrix methods are rewritten by $J_c^{(TMM-S)} = 0$ and $J_c^{(TMM-H)} = 0$, in which $J_c^{(TMM-S)}$ is the LHS of Eq. (4.27) of Ref. [2], and $J_c^{(TMM-H)}$ is the LHS of Eq. (14) of Ref. [19]. Figure 3 shows the characteristic function of the present method and two transfer matrix methods, J_c, $J_c^{(TMM-S)}$, and $J_c^{(TMM-H)}$, for the electron energy from 0 to 1.2 eV. The solutions of the energy equations are found at the valley approaching zero. From the references, we see that $J_c^{(TMM-S)}$ does not include the term of $\exp(iKL)$, but $J_c^{(TMM-H)}$ does. However, for a given electron energy, we can obtain two values of $\exp(iKL)$, denoted by $\exp(iKL)^{(+)}$ and $\exp(iKL)^{(-)}$. Thus, we have two different values of $J_c^{(TMM-H)}$, marked by $J_c^{(TMM-H)(+)}$ and $J_c^{(TMM-H)(-)}$, respectively relative to $\exp(iKL)^{(+)}$ and $\exp(iKL)^{(-)}$ for each energy shown in Fig. 3. Since the eigenfunction is decaying with the increase of the distance from the surface, the absolute value of $\exp(iKL)$ should be less than one. Thus the solutions of the energy equation, $J_c^{(TMM-H)} = 0$, corresponding to the function of $\exp(iKL)$ in the condition $|\exp(iKL)| > 1$ are spurious solutions. For TMM-S, although $\exp(iKL)$ does not appear in the energy equation, the solved roots also include spurious solutions. The reference offers another criterion. If we rewrite the LHS of the checking function given in Eq. (4.29) of Ref. [2] as Γ, the solutions for the surface modes exist under the

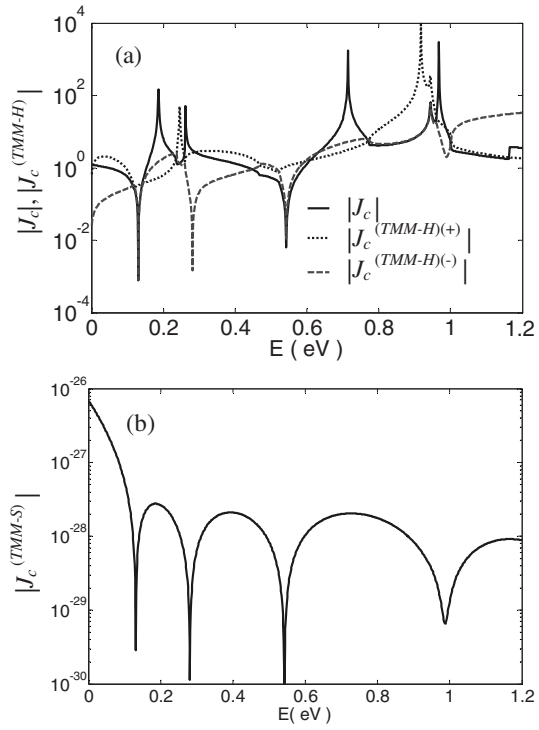

FIG. 3. The absolute values of characteristic functions for the terminated biperiodic superlattice, in each cell of which d_1=4 nm, d_2=d_3=d_4=2 nm, x_1=x_3=0, and x_2=x_4=0.5. (a) The absolute values of J_c, $J_c^{(TMM-H)(+)}$, $J_c^{(TMM-H)(-)}$. J_c is used to obtain the surface states for the present method and $J_c^{(TMM-H)(+)}$ and $J_c^{(TMM-H)(-)}$ are used for TMM-H. (b) The absolute values of $J_c^{(TMM-S)}$, which is used to obtain the surface states for TMM-S.

condition $|\Gamma|>1$. The absolute values of $\exp(iKL)^{(+)}$, $\exp(iKL)^{(-)}$, and Γ are shown in Fig. 4. According to the results of Figs. 3 and 4, we find that the root E=0.2808 eV for TMM-H is the spurious solution since the absolute value of $\exp(iKL)$ for the solution is greater than 1. For TMM-S,

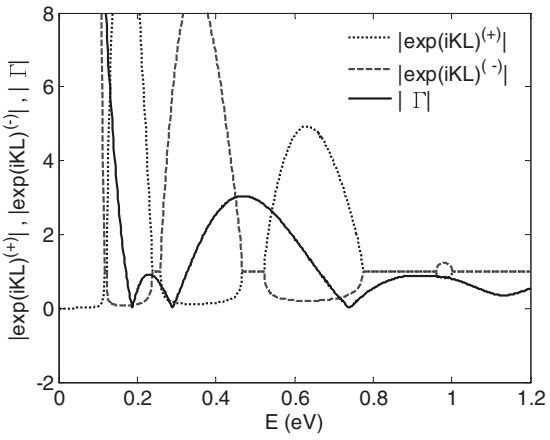

FIG. 4. The absolute values of $\exp(iKL)(+)$, $\exp(iKL)(-)$, and Γ for the electron energy from 0 to 1.2 eV in the biperiodic superlattice. To obtain the correct surface states, it is required to remove the spurious roots according to the values of Γ for TMM-S, and $\exp(iKL)(+)$ and $\exp(iKL)(-)$ for TMM-H.

TABLE I. Calculated energy for the electron surface states in a four-layer $Al_xGa_{1-x}As$ superlattice terminated by AlAs. In each cell, the width in each layer is d_2=d_3=d_4=2 nm. The Al concentration in each layer is x_1=x_3=0, x_2=x_4=0.5.

	This method	TMM-H		TMM-S	
d_1	E (eV)	E (eV)	$\lvert e^{iKL}\rvert$	E (eV)	$\lvert\Gamma\rvert$
4 nm	0.1307	0.1307	0.1675	0.1307	5.9655
	0.5426	0.2808[a]	4.7602	0.2808[a]	0.2094
		0.5426	0.3802	0.5426	2.6267
2 nm	none	0.3216[a]	1.0649	0.2454[b]	1.0013
				0.3216[a]	0.9768
				0.9178[b]	1.0001

[a]Spurious solutions.
[b]Incorrect solutions.

since the absolute value of Γ for the solution E=0.2808 eV is less than 1, both solutions are spurious ones. However, spurious solutions are not included in the results of the present method. Table I shows all of the solutions gained by the present method and compares the transfer matrix methods for the four-layer superlattice with different bases in each cell. We see the solutions calculated by TMM-H and TMM-S include the spurious solutions for various cases but the present method does not. Moreover, some incorrect solutions occur in the results by TMM-S because of the numerical truncation in the computation. The numerical results show that it is straightforward to accurately calculate the surface modes of superlattices by the present theory. But, the problems of incorrect solutions or numerical overflow may occur in traditional methods.

Next, we study the numerical implementation for a chirped $Al_xGa_{1-x}As$ superlattice terminated by a surface of

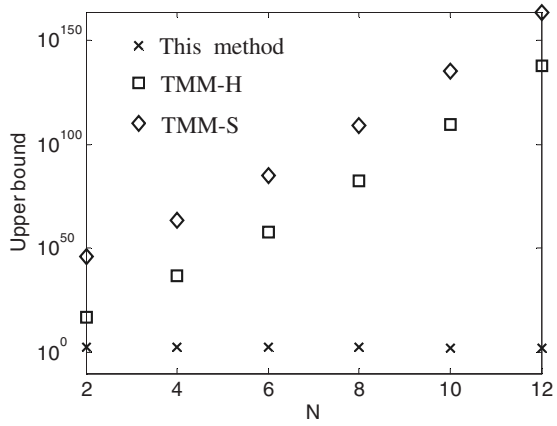

FIG. 5. The upper bounds of the calculation for surface states in the N-layer chirped superlattice by TMM-H, TMM-S, and the present methods. The absolute values of J_c, f_s, g_s, and h_s for the present method, $J_c^{(TMM-H)}$, $m_{i,j}^{(TMM-H)}$, and $\exp(ikL)$ for TMM-H, and $J_c^{(TMM-S)}$, $m_{i,j}^{(TMM-S)}$, and Γ for TMM-S are calculated to determine the surface states.

AlAs, in which the Al concentration of each odd layer is 0 and that of each even layer is 0.5. For each period, the width of each layer is $d_{s,n}=30[1+(n/N)]nm$. The present method and both transfer matrix methods are also applied to solve the surface modes for the structure with N being changeable from 2 to 12. From Eq. (3), we see that the eigenvalue equations used by the present method are in terms of f_s, g_s, and h_s. However, by the transfer matrix methods, the eigenvalue equations are expressed by each element of the global matrix, $m_{i,j}^{(TMM)}$ for $i,j=1,2$. Further, since spurious solutions are included in the solved results of the transfer matrix methods, the spurious solutions need to be removed according to the absolute value of $\exp(iKL)$ for TMM-H and Γ for TMM-S. The upper bounds of the calculation for the surface states in the superlattice by these three methods are shown in Fig. 5. The numerical results of Fig. 5 show that using the surface states equations in the present method to calculate the surface states leads to a better stability property than using the transfer matrix methods.

In conclusion, we have proposed a graph method to determine the electronic surface states in a complex basis superlattice terminated by the surface and a multilayer clad barrier. This method has some added benefits compared to traditional methods. First, based on the present expressions, it is convenient to calculate each term of the equations without recursive calculation or numerical overflow. Moreover, the roots solved by the present method do not include spurious ones. However, calculation of the surface states by the traditional methods may cause incorrect results or numerical instability for complex basis superlattices.

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[1] J. Kłos and H. Puszkarski, Phys. Rev. B **68**, 045316 (2003).
[2] M. Stęślicka, R. Kucharczyk, A. Akjouj, B. Djafari-Rouhani, L. Dobrzynski, and S. G. Davison, Surf. Sci. Rep. **47**, 93 (2002).
[3] W. Trzeciakowski, Phys. Rev. B **38**, 12493 (1988).
[4] W. L. Bloss, Phys. Rev. B **44**, 8035 (1991).
[5] S. Fafard, Phys. Rev. B **50**, 1961 (1994).
[6] D. Indjin, V. Milanović, and Z. Ikonić, Phys. Rev. B **52**, 16762 (1995).
[7] X. H. Wang, B. Y. Gu, G. Z. Yang, and J. Yang, Phys. Rev. B **58**, 4629 (1998).
[8] J. Klos, Phys. Status Solidi B **242**, 1399 (2005).
[9] D. W. L. Sprung, P. Jagiello, J. D. Sigetich, and J. Martorell, Phys. Rev. B **67**, 085318 (2003).
[10] H. K. Sy and T. C. Chua, Phys. Rev. B **48**, 7930 (1993).
[11] S. D. Chen, C. Narayan, and A. S. Karakashian, Physica B **228**, 239 (1996).
[12] P. Pereyra, Ann. Phys. **320**, 1 (2005).
[13] S. Y. Ren, Phys. Rev. B **64**, 035322 (2001).
[14] A. Patanè, D. Sherwood, L. Eaves, T. M. Fromhold, M. Henini, P. C. Main, and G. Hill, Appl. Phys. Lett. **81**, 661 (2002).
[15] V. Lousse and S. Fan, Phys. Rev. B **72**, 075119 (2005).
[16] A. Mayer, Phys. Rev. E **74**, 046708 (2006).
[17] B. Brzostowski and R. Kucharczyk, Phys. Rev. B **67**, 125305 (2003).
[18] I. Bartoš, T. Strasser, and W. Schattke, Prog. Surf. Sci. **74**, 293 (2003).
[19] W. Q. Huang, K. Q. Chen, Z. Shuai, L. Wang, and W. Hu, Phys. Lett. A **325**, 70 (2004).
[20] W. J. Hsueh, J. C. Lin, and H. C. Chen, J. Phys.: Condens. Matter **19**, 266007 (2007).
[21] W. Mayeda, *Graph Theory* (Wiley, New York, 1972).