Calculated defect states in semiconductor superlattices within a tight-binding model

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The localized states which appear in a superlattice as a result of thickness variations of barriers or quantum wells are calculated in the framework of the tight-binding approximation. We obtain very simple formulas in terms of single-quantum-well parameters. There is always a localized state for an enlarged or narrowed quantum well. Two localized states exist in the case of decreased barrier thickness. The range of validity of the formulas is discussed as a function of the superlattice period.

I. INTRODUCTION

The semiconductor heterointerfaces of superlattices (SL's) grown by molecular-beam epitaxy consist of islands between which the interface position changes by one or two monolayers.[1,2] On the other hand, enlarged quantum wells (QW's) can be intentionally introduced in SL's. Such structures, where the QW plays the role of probe, were used, for example, to study so-called "perpendicular" transport.[3] It is important in both cases to know the localized states which occur when an enlarged or narrowed QW or barrier is introduced in a SL. Of course, when the defects are not introduced intentionally, their lateral size is limited and the binding energy depends on the size. We will consider only the case where the lateral size is large enough to be considered infinite. The calculation is then a one-dimension calculation.

Combescot and Benoit à la Guillaume have calculated the binding energy of an electron localized on a defect for an enlarged quantum well,[4] and Gashimzade, Ivchenko, and Kosobukin[5] have calculated the same for a more general imperfection of the periodicity. The calculation was done in the framework of the transfer-matrix theory. The final expressions of the binding energy are very general but rather complicated.

The purpose of this paper is to establish simple analytical formulas with which one can calculate the energy levels of the states introduced by the defects. The formulas are obtained in the framework of the tight-binding approximation. We discuss their range of validity as a function of the number of monolayers (ML) in the QW or the barrier in the SL.

II. THEORY

We consider a sequence of alternating QW's and barriers which may have different thicknesses. In the tight-binding approximation,[6,7] the wave function of the fundamental level is written

$$\chi^k(z)=\frac{1}{\sqrt{N}}\Psi_n^k\varphi_n(z) .$$

z is the growth axis, and φ_n is the fundamental state of the nth QW when the QW is considered as isolated. The summation is done on the N QW's.

Let us now consider a SL. The thicknesses of the wells and barriers are L and h, respectively. The period is $d=L+h$. We keep only nearest-neighbor interactions. The eigenvalue E is written as a solution of the following equation:

$$E\Psi_n^k+\frac{I}{2}(\Psi_{n+1}^k+\Psi_{n-1}^k)=E_c\Psi_n^k , \tag{1}$$

where $E_n=E_c$ is the confinement energy in the nth QW. The transfer integral I is defined as

$$\frac{I}{2}=-\int_{-\infty}^{+\infty}\varphi(z)V(z)\varphi(z-d)dz ,$$

where $V(z-nd)=-V$ if $|z-nd|\le(L/2)$ and $V=0$ if $|z-nd|>(L/2)$.

The well-known solution of Eq. (1) is obtained by writing $\Psi_n^k=e^{iknd}$. Then,

$$E(k)=E_c-I\cos kd .$$

Let us consider a SL which contains a "defect" characterized by a modified confinement energy, δE of the QW for $n=0$ and modified transfer integrals $\delta I_{0,-1}$ and $\delta I_{0,+1}$ with the neighboring QW's, $n=\pm1$. Taking the energy origin as $E_c=0$, we obtain

$$E_n=\delta E\delta_n ,$$

$$\delta I_{n+1,n}=\delta I_{n,n+1}=\delta I_r\delta_n+\delta I_l\delta_{n+1} ,$$

$$\delta I_{n-1,n}=\delta I_{n,n-1}=\delta I_l\delta_n+\delta I_r\delta_{n-1} ,$$

where δI_r and δI_l are the differences of the transfer integrals with the right and left neighbors, respectively. δ_n is the Kronecker symbol.

Equation (1) becomes

$$E\Psi_n+\frac{I}{2}(\Psi_{n+1}+\Psi_{n-1})$$

$$=\left[\delta E\Psi_0-\frac{\delta I_r}{2}\Psi_{+1}-\frac{\delta I_l}{2}\Psi_{-1}\right]\delta n$$

$$-\frac{\delta I_l}{2}\Psi_0\delta_{n+1}-\frac{\delta I_r}{2}\Psi_0\delta_{n-1} .$$

In our analysis we use the local perturbation method developed by Lifshitz.[8,9] Let us introduce the Green function

$$g(n-n')=\int_0^{\pi}\frac{d(kd)}{\pi}\frac{e^{i(n-n')kd}}{E+I\cos kd}\ .$$

The coefficient Ψ_n can be written

$$\Psi_n=g(n)\left\{\delta E\Psi_0-\frac{\delta I_r}{2}\Psi_{+1}-\frac{\delta I_l}{2}\Psi_{-1}\right\}-\left\{g(n+1)\frac{\delta I_l}{2}+g(n-1)\frac{\delta I_r}{2}\right\}\Psi_0\ .$$

We obtain a three-equation system:

$$\Psi_0\left\{1+\frac{g(1)}{2}(\delta I_l+\delta I_r)-\delta E g(0)\right\}+\frac{g(0)}{2}(\delta I_r\Psi_{+1}+\delta I_l\Psi_{-1})=0\ ,$$

$$\Psi_{+1}\left\{1+\frac{g(1)}{2}\delta I_r\right\}-\Psi_0\left\{g(1)\delta E-g(2)\frac{\delta I_l}{2}-g(0)\frac{\delta I_r}{2}\right\}+\Psi_{-1}g(1)\frac{\delta I_l}{2}=0\ ,$$

$$\Psi_{-1}\left\{+\frac{g(1)}{2}\delta I_l\right\}-\Psi_0\left\{g(1)\delta E-g(0)\frac{\delta I_l}{2}-g(2)\frac{\delta I_r}{2}\right\}+\Psi_{+1}g(1)\frac{\delta I_r}{2}=0\ .$$

The two first Green functions are

$$Ig(0)=\frac{\mathrm{sgn}(\varepsilon)}{\sqrt{\varepsilon^2-1}}\ ,$$

$$Ig(1)=1-\frac{\varepsilon\,\mathrm{sgn}(\varepsilon)}{\sqrt{\varepsilon^2-1}}$$

where $\varepsilon=E/I$ and $\varepsilon^2>1$.

Let us now consider separately the cases where the thickness of the QW or barrier is varied. For an enlarged or narrowed QW, $\delta I_r=\delta I_l=0$. The solution is given by

$$1-g(0)\delta E=0\ .$$

There is always a localized state, the energy of which is

$$\varepsilon=\sqrt{1+e^2}\,\mathrm{sgn}(e) \tag{2}$$

where

$$e=\delta E/I\ .$$

As Fig. 1 shows, the energy level is lower or higher than the energy band, accordingly as the QW thickness is enlarged or narrowed, respectively.

For an enlarged or narrowed barrier, $\delta E=\delta I_l=0$. E is solution of the equation

$$1+g(1)\delta I+[g^2(1)-g^2(0)]\left[\frac{\delta I}{2}\right]^2=0\ .$$

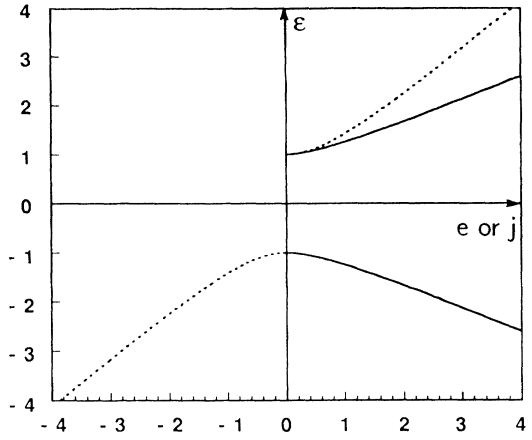

FIG. 1. The solid line is the localized state energy as a function of the difference between energy confinements in the modified QW and the QW's in the SL:

$$\varepsilon=\sqrt{1+e^2}\,\mathrm{sgn}(e)\ .$$

The dotted line is the localized state energy as a function of the difference between transfer integrals through the modified barrier and through barriers in the SL:

$$\varepsilon=\pm\frac{(1+2/j)^2+1}{(1+2/j)^2-1}\ ,$$

All the energies are taken in units of the transfer integral in the SL.

Let us note $j=\delta I/I$. There is no localized state for $-1<j<0$, i.e., for an enlarged barrier. There are two solutions for $j>0$, i.e., for a narrowed barrier:

$$\varepsilon=\pm\frac{(1+2/j)^2+1}{(1+2/j)^2-1}\ . \tag{3}$$

Figure 1 shows the variation of ε as a function of j. The two solutions correspond to the symmetric and antisymmetric linear combinations of the wave function centered on the QW's adjacent to the barrier.

In order to estimate the range of validity of formulas (2) and (3), we have compared results obtained in this model with results obtained in a computer calculation using matrix transfer formalism. The calculation is done for a variation of the QW or barrier thickness of 1 ML in a GaAs/AlAs SL. The absolute values of energy found in our model are always larger than the absolute values calculated with the matrix transfer model. The accuracy of the formulas for Γ electrons, for a thickness variation of either the QW or the barrier, is found to be better than 10% in SL's where the period is larger than 13–15 ML and the barrier thickness is equal to or larger than 2 ML. The accuracy is even better for heavy holes or X electrons

which have heavy masses. In this model, the energy levels are given as a function of the confinement energy in an isolated QW and the transfer integral between two QW's. These parameters are easily obtained as a function of QW and barrier thicknesses with a simple pocket-calculator computation. In real SL's, one would have to take into account an energy-dependent mass for electrons and valence-band mixing for holes.

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