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Nature of the extended states in random dimer-barrier superlattices

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Abstract

We theoretically study electron transmission in intentionally disordered GaAs–$Al_xGa_{1-x}As$ superlattices with structural short-range correlations in the Al mole fraction of the $Al_xGa_{1-x}As$ layers. The Al mole fraction in the equal-width $Al_xGa_{1-x}As$ layers takes at random two different values, but with the constraint that one of them only appears at random in pairs, while GaAs layers are identical. We demonstrate that the superlattice supports two types of extended states, one of them comes from resonance effects at *dimer* barriers, as it was already reported for random *dimer* well superlattices, while the other type arises as a consequence of the binary nature of this heterostructure. Conditions for their observation in transport experiments are discussed.

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1. Introduction

The theory of one-parameter scaling, earlier introduced in Ref. [1], led to the general belief that all one-particle states in disordered systems were exponentially localized in one and two dimensions (see Refs. [2,3] for a comprehensive review). Later advances in nanotechnology made it possible to grow artificial semiconductor superlattices (SLs) with tailored physical properties and open the possibility to experimentally verify former theoretical predictions. In particular, Chomette et al. [4] claimed that Anderson localization [5] was responsible for the increase of the photoluminescence intensity observed in intentionally disordered SLs.

However, since the beginning of the 1990s, several works showed that a band of delocalized states appears in one-dimensional tight-binding Hamiltonians with correlated diagonal and/or off-diagonal terms [6–10]. A more dramatic occurrence of electron delocalization arises in Kronig–Penney models with dimer impurities since there exist infinitely many bands of delocalized states [11]. Later, Diez et al. conjectured that GaAs–$Al_xGa_{1-x}As$ SLs with *dimer* wells placed at random, referred to as DWSL, might exhibit high DC-conductance [12–14]. Such a DWSL consists

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of a number of GaAs quantum wells of two different thicknesses placed at random, with the additional constraint that one of them always appears in pairs (*dimer* well). Roughly speaking, resonances at specific energies arise due to the occurrence of paired wells and, most importantly, these resonances survive even if dimer wells are randomly distributed. Few years after this proposal, suppression of localization by correlations was further put forward for the explanation of the observed transport properties and high DC-conductance of GaAs–$Al_xGa_{1-x}As$ DWSLs [15].

In this work we consider an SL where two $Al_xGa_{1-x}As$ barriers of different Al mole fractions are introduced at random in the SL, but one of them can only appear in pairs. This heterostructure will be referred to as *dimer* barrier SL, (DBSL) hereafter. Besides the similarity with the formerly introduced DWSL, we will show below that two types of extended electronic states arise. One of them comes from the already-mentioned resonance effect. The other one is solely due to the binary nature of the composition of the SL even in the absence of correlated disorder.

2. Model

Electronic states close to the conduction-band edge with vanishing momentum parallel to the layers are successfully described by the envelope-function approximation [16]. Assuming that all the barriers are of the same thickness (d_b), we are then faced with a Ben Daniel–Duke model where barrier energies V_n ($n = 1, \ldots, N$, where N is the number of barriers in the DBSL) form a random sequence of two values, V and $\bar{V}$. These two energies are proportional to the two possible values of the Al mole fraction in the $Al_xGa_{1-x}As$ barriers, x, for $x \leqslant 0.45$. The sequence of energies is short-range correlated since $\bar{V}$ only appears forming pairs (see Fig. 1). At the contacts of the DBSL, the envelope function takes the form

$$\chi(z) = \begin{cases} e^{i\kappa z} + r_N\, e^{-i\kappa z}, & z < z_1 - d_b/2, \\ t_N\, e^{i\kappa z}, & z > z_N + d_b/2, \end{cases} \tag{1}$$

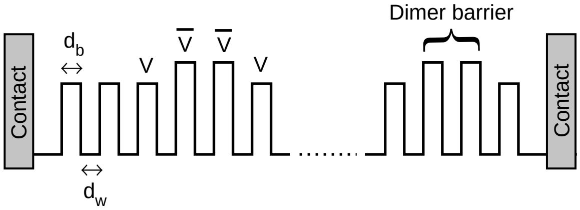

Fig. 1. Schematic view of the conduction band-edge profile of the DBSL, where pairs of $\bar{V}$ barriers appear at random.

where z_n denotes the coordinate along the growth direction of the center of the nth barrier, $\kappa^2 \equiv 2m_w E/\hbar^2$ and m_w is the electron effective-mass in GaAs. Here t_N and r_N are the transmission and reflection amplitudes of the SL. The knowledge of the 2×2 transfer matrix of the DBSL, $M(N)$, allows us to relate t_N and r_N in a closed expression, namely $M_{11}(N) = 1/t_N^*$ and $M_{12}(N) = r_N/t_N$. The SL can be regarded as an array of building blocks, each block formed by an $Al_xGa_{1-x}As$ layer along with the two adjacent GaAs half-layers. Therefore, $M(N) \equiv \prod_{n=N}^{1} P_n$ and the transfer matrix P_n of each block reads [17]

$$P_n \equiv \begin{pmatrix} \alpha_n & \beta_n \\ \beta_n^* & \alpha_n^* \end{pmatrix}, \tag{2}$$

whose elements are given by

$$\alpha_n = \left[\cosh(\eta_n d_b) + \frac{i}{2}\left(\frac{m_{b,n}\kappa}{m_w\eta_n} - \frac{m_w\eta_n}{m_{b,n}\kappa}\right)\sinh(\eta_n d_b)\right] \times e^{i\kappa d_w} \tag{3a}$$

$$\beta_n = -\frac{i}{2}\left(\frac{m_{b,n}\kappa}{m_w\eta_n} + \frac{m_w\eta_n}{m_{b,n}\kappa}\right)\sinh(\eta_n d_b)e^{-i\kappa d_w}, \tag{3b}$$

where $\eta_n^2 \equiv 2m_{b,n}(V_n - E)/\hbar^2$. Two values are allowed, η and $\bar{\eta}$, corresponding to barrier heights V and $\bar{V}$, respectively. We take into account the variation of the effective mass with the Al mole fraction. Thus, the effective mass in the nth barrier $m_{b,n}$ can take the values m_b and $\bar{m}_b$, corresponding to barrier heights V and $\bar{V}$, respectively.

3. Extended states

It has been shown in the case of DWSL [13] that there exists an extended state when $\mathrm{Re}(\alpha_d) = 0$ and

$|\mathrm{Tr}(P_r)| \leqslant 2$, where

$$\alpha_d = \left[\cosh(\eta d_b) + \frac{i}{2}\left(\frac{m_b\kappa}{m_w\eta} - \frac{m_w\eta}{m_b\kappa}\right)\sinh(\eta d_b)\right] e^{i\kappa\bar{d}_w},$$

$\bar{d}_w$ being the width of each quantum well forming the dimer, and P_r is the transfer matrix of each building block in a regular SL (i.e., $V_n = V$). In a straightforward manner, it is easy to demonstrate that similar conditions hold in the case of DBSL. In the latter, conditions for the existence of an extended state turn out to be formally the same, but now

$$\alpha_d = \left[\cosh(\bar{\eta} d_b) + \frac{i}{2}\left(\frac{\bar{m}_b\kappa}{m_w\bar{\eta}} - \frac{m_w\bar{\eta}}{\bar{m}_b\kappa}\right)\sinh(\bar{\eta} d_b)\right] \times e^{i\kappa d_w}. \tag{4}$$

The following equations can be derived from these conditions:

$$|\cosh(\eta d_b)\cos(\kappa d_w) - \xi_- \sinh(\eta d_b)\sin(\kappa d_w)| \leqslant 1, \tag{5a}$$

$$\cosh(\bar{\eta} d_b)\cos(\kappa d_w) - \bar{\xi}_- \sinh(\bar{\eta} d_b)\sin(\kappa d_w) = 0 \tag{5b}$$

for energies below the lowest barrier. For brevity we have defined

$$\xi_\pm \equiv \frac{1}{2}\left(\frac{m_b\kappa}{m_w\eta} \pm \frac{m_w\eta}{m_b\kappa}\right),$$

$$\bar{\xi}_\pm \equiv \frac{1}{2}\left(\frac{\bar{m}_b\kappa}{m_w\bar{\eta}} \pm \frac{m_w\bar{\eta}}{\bar{m}_b\kappa}\right).$$

Similar equations can be found for energies above the lowest barrier; we consider only the former case for the sake of simplicity. The energy for which the last two conditions hold simultaneously (if exists) corresponds to an extended state in a regular SL with a single dimer barrier, and it will be referred to as *dimer* resonance energy, E_d. It can be shown numerically that, in fact, this energy corresponds to an extended state for an SL with a randomly distributed ensemble of dimers.

Unexpectedly, the DBSL supports another type of extended state, its origin being completely different. Let us take a system built with two kinds of blocks distributed randomly on a chain. It is evident that the effects of randomness will be removed when, for a *given* electron energy, the positions of two consecutive different blocks can be interchanged. In this case, all the blocks of each type can be moved to one of the two sides. This argument can be mapped to the case of an SL using the transfer matrix formalism, assuming that each block corresponds to an SL period. Thus the condition for the randomness removing reduces to that of the commutation of the transfer matrices corresponding to the unit block formed by two types of barriers $[P, \bar{P}] = 0$. This leads to the following equations:

$$\mathrm{Im}(\beta\bar{\beta}^*) = 0, \tag{6a}$$

$$\bar{\beta}\,\mathrm{Im}(\alpha) = \beta\,\mathrm{Im}(\bar{\alpha}). \tag{6b}$$

In the case of the DBSL, these equations can be fulfilled simultaneously, for Eq. (6a) reduces to an identity, whereas Eq. (6b) yields the following transcendental equation:

$$\frac{\xi_+ \sinh(\eta d_b)}{\bar{\xi}_+ \sinh(\bar{\eta} d_b)} = \frac{\cosh(\eta d_b)\sin(\kappa d_w) + \xi_- \sinh(\eta d_b)\cos(\kappa d_w)}{\cosh(\bar{\eta} d_b)\sin(\kappa d_w) + \bar{\xi}_- \sinh(\bar{\eta} d_b)\cos(\kappa d_w)}. \tag{7}$$

In order to have an extended state, the energy at which randomness effects are removed must lie within the minibands of the regular SL (formed by barriers of only one type)

$$|\mathrm{Tr}(P)| \leqslant 2, \quad |\mathrm{Tr}(\bar{P})| \leqslant 2. \tag{8}$$

The energy E_c obtained by solving Eqs. (7) and (8) will be referred to as *commuting* resonance energy hereafter.

4. Numerical results

To ascertain whether the energies given by expressions (5) and (7) correspond to truly extended states or not, we have performed a numerical study. We show in Fig. 2 the transmission coefficient for a DBSL made of GaAs–$Al_xGa_{1-x}As$ with the following structural parameters: $d_b = 25$ Å, $d_w = 25$ Å, $x = 0.3$ and $\bar{x} = 0.44$, where x and $\bar{x}$ stand for the Al mole fractions at the lowest and the highest barriers, respectively. The fraction of *dimer* barriers was chosen to be

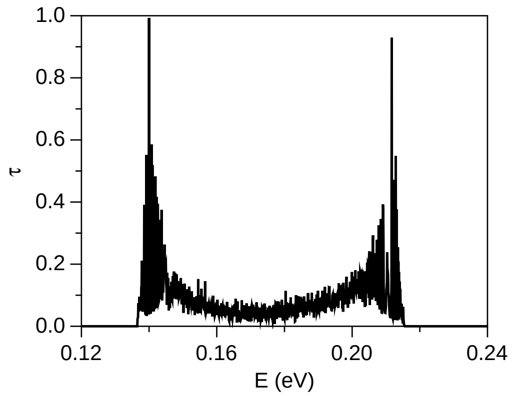

Fig. 2. Transmission coefficient as a function of energy for a DBSL with $d_b = 25$ Å, $d_w = 25$ Å, $x = 0.3$, $\bar{x} = 0.44$ and $N = 1000$ periods. The fraction of dimer barriers is 30%. Two resonances can be seen at $E = E_d \simeq 0.140$ eV and $E = E_c \simeq 0.212$ eV.

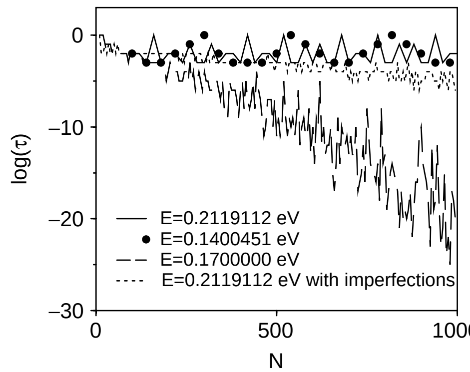

Fig. 3. Dependence of the transmission coefficient on the system size (number of periods N). (—) and (•) correspond to E_c and E_d, respectively, whereas (----) corresponds to $E = 0.170$ eV. The (· · · · ·) corresponds to the unintentionally disordered SL at E_c, where the widths of barriers and wells fluctuate 1% around their mean values.

30%. With these parameters, it can be seen that two resonances appear at the edges of the miniband. The energies at which these resonances appear turn out to be those obtained by solving Eqs. (5) and (7). The solutions are $E_d \simeq 0.140$ eV and $E_c \simeq 0.212$ eV for the *dimer* resonance and the *commuting* resonance, respectively. We represent in Fig. 3 the dependence of the transmission coefficient on the system size for various energies. It can be seen that the curves for E_d and E_c have zero slope, indicating an infinite localization length. Meanwhile, far away from the resonances, we observe that the states display a nonzero finite localization length. Thus, we suggest that the energies obtained from Eqs. (5) and (7) correspond in fact with two different kinds of extended states. The effect of unintentional disorder on these resonances can also be observed.

In order to check the applicability of the present results in actual SLs, where some degree of unintentional disorder due to interface roughness is unavoidable, we also allow wells and barriers to fluctuate randomly (see Ref. [13] for further details of the model of interface roughness). The width of the various layers is chosen $d_x(1 + W\varepsilon)$, where $d_x = d_b$, d_w is the nominal width, W is a dimensionless parameter measuring the degree of unintentional disorder and ε denotes a random number distributed uniformly between $-\frac{1}{2}$ and $\frac{1}{2}$. Fig. 3 shows that the interface roughness makes the electronic state corresponding to the *commuting* resonance to become localized. Here $W = 0.03$, i.e., average fluctuations are of the order of 1% of the layer width. However, the localization length is still large enough to allow a clear experimental validation of the existence of these phenomena in high-quality SLs.

We would like to point out that the kind of *commuting* extended states we are describing are not characteristic of dimer SLs in the sense that no dimer correlations are needed at all. It means that an SL with a binary distribution of barrier heights satisfying the following correlator $\langle V_n V_m \rangle = V^2 \delta_{nm}$, should exhibit the same kind of extended state. Thus, it is important to emphasize that we have found a system in which two kinds of extended states are supported, their origins being completely different: one of them due to short-range correlations and the other coming from the commuting nature of the transfer matrices describing the system at certain energies.

Actually, the *commuting* extended states we are describing seem to appear in a number of binary models. For instance, similar conditions to that found in the case of a DBSL can be obtained for DWSLs. In this SL, it can be found that a new resonance arises when the condition

$$\kappa(\bar{d}_{\rm w} - d_{\rm w}) = \pi n \tag{9}$$

is fulfilled. Here n is an integer, and $\bar{d}_{\rm w}$ and $d_{\rm w}$ are the widths of two types of quantum wells in the DWSL, respectively. Another example of this kind of resonance, can be found in the random binary Kronig–Penney model with delta barriers. In this model the *commuting* conditions (6a) and (6b) lead to the same resonant energy observed by Ishii [18], and discussed by Hilke and Flores [19], for a set of δ barriers with randomly distributed heights. Extended states due to different mechanisms in some other kinds of binary SLs [20] and binary alloys [21] have been reported so far.

5. Final remarks

To conclude, a few words are in order regarding the possible observation of these two types of extended states in intentionally disordered SLs. We have already demonstrated that extended states in DWSLs manifest themselves in transport measurements at low temperature [15]. In particular, DC resistance of DWSLs with a suitable selection of parameters and ordered (periodic) SLs GaAs–$Al_xGa_{1-x}As$ show a *plateau* at low temperature, whereas this *plateau* is absent when the *dimer* constraint is relaxed (i.e., SLs with two types of quantum wells placed at random without pairing). We conjecture that the same measurements can be performed in DBSLs to ascertain the truly extended character of the *commuting* extended states which, in this kind of SLs, are easier to locate within the miniband. However, DC measurements should probably be unable to separate the effects of both types of extended states. Thus, after carefully selecting the growing parameters of the SLs, it is possible to place the *dimer* resonant energy out of the band so that transport properties come only from *commuting* extended states. Though, as noticed previously, dimer correlations are not needed to find *commuting* states, this way of constructing the SL will clarify the role of these extended states in intentionally disordered SLs.

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