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Multiband coupling and electronic structure of short-period (GaAs)$_n$//(AlAs)$_n$ (001) superlattices

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Abstract. It is shown that effective mass approximation together with short range interface corrections can be used to calculate short-period abrupt (GaAs)$_n$//(AlAs)$_n$ (001) superlattices. The results obtained are in excellent agreement with results of pseudopotential calculations (A. Zunger et al.) in a wide range of superlattices periods (from \( n = 1 \) to \( n = 20 \)).

Introduction

Short-period (GaAs)$_n$//(AlAs)$_n$ (001) semiconductor superlattices (SL) is a convenient model for theoretical and experimental analysis of transformation of heterostructure type from type I to type II. Depending on the number of monolayers, the conduction band minimum of SL is mainly formed either by \( \Gamma_1 \) state of the conduction band of GaAs or by \( X_1 \) state of the conduction band of AlAs.

In a series of recent publications [1–4] pseudopotential method was used for direct numerical calculations of electronic structure of (GaAs)$_n$//(AlAs)$_n$ (001) SL. However possibility of using of the effective mass approximation (EMA) to analyze short-period abrupt SL was questioned due to absence of interband coupling in that theory. Nevertheless, it was shown by Burt in [5] that this coupling is taken into account in the standard Luttinger–Kohn envelope-function theory and mainly arises due to rapid change of potential at the interface. In the framework of the EMA this coupling gives rise to short range interface corrections (SRIC) in effective Hamiltonian, which modify interface boundary conditions for envelope functions and lead to interband and intraband coupling of the states. Coefficients of this coupling can be determined from a microscopic theory or introduced phenomenologically.

For GaAs/AlAs (001) interface SRIC were analyzed in [6–10]. However, up to the present time there is a lack of unified opinion concerning the coupling coefficients. According to [6–7] these corrections lead only to \( \Gamma_{5x} - \Gamma_{15y} \) coupling in the valence band and to \( \Gamma_1 - X_{3z}, X_{1x} - X_{1y} \) and \( X_{3x} - X_{3y} \) couplings in the conduction band. In contrast to these results, analysis of pseudopotential Hamiltonian [8] shows that \( X_{1x} - X_{1y} \) coupling is zero and \( X_{1z} - X_{3z} \) coupling is non-zero. In [9], where tight binding model was used, it was shown that \( \Gamma_1 - X_{1z} \) coupling can exist only when there are some interface imperfections. However magnetotunneling measurements [10] indicate that both \( X_1 \) and \( X_3 \) bands contribute to the \( \Gamma - X_z \) and \( X_x - X_y \) couplings.

In the present work the EMA together with SRIC (EMA + SRIC model) was for the first time used for systematic analysis of short range corrections that arise at GaAs/AlAs (001) interface. Using the method of invariants in \( T_d^2 \) space-group, we obtained 7-band \( \Gamma_1 \oplus \ast X_1 \oplus \ast X_3 \) and 6-band \( \Gamma_8 \oplus \Gamma_7 \) multiband effective Hamiltonians, which include SRIC in all orders of perturbation theory. These Hamiltonians were used to calculate electronic structure of short-period (GaAs)$_n$//(AlAs)$_n$ (001) SL. Comparing our results with the results of pseudopotential calculations [2, 4] we determined the coupling coefficients.
It was shown that when one takes into account the short range corrections in the framework of the EMA+SRIC model it allows one to adequately describe energy structure of electron and oscillating character of $\Gamma-X$ anticrossing in the whole range of studied SL periods (from $n = 1$ to $n = 25$).

1. Multiband coupling in effective Hamiltonians

Hamiltonian of $A_3B_5$ heterostructure with single heterointerface $AB/A'B$ can be presented in the following form

$$ H = \frac{p^2}{2m_0} + \frac{1}{2} [U_2(x) + U_1(x)] + f[n(x - a)]\Delta U(x). \quad (1) $$

Here $U_{1,2}(x)$ are the crystal potentials on the left and right sides of the interface respectively, which have the same period and symmetry; $f[n(x - a)]$ is an odd step-function, modulating periodic potential; $n$ is a unit vector normal to the interface; $a$ is Bravais lattice vectors determining positions of atom B at the interface plane.

In the framework of the EMA+SRIC model multiband Hamiltonian contains the following SRIC terms

$$ H_{n_1,m_1}^{(\alpha_0)\beta} (x) = \{ \alpha, n, k_{\alpha_0}^0 \} |f[n(x - a)]\Delta U(x)|\beta, m, k_{\beta}^0 \} \delta[n(x - a)]. \quad (2) $$

Here $|\alpha, n, k_{\alpha_0}^0 \}$ and $|\beta, m, k_{\beta}^0 \}$ are Bloch states, which correspond to $k_{\alpha}^0$ and $k_{\beta}^0$ points of the Brillouin zone of a virtual Ga$_{0.5}$Al$_{0.5}$As crystal; $\alpha$ and $\beta$ denotes bands (including irreducible representations of the space-group $T_d^2$). Matrix element in the right hand side of Eq. (2) determines coefficients of interband and intraband couplings. Since $\Delta U(x)$ is an invariant in the translation group, non-zero contribution into the coupling of these states is produced only by the following rapid Fourier oscillations of $f[n(x - a)]$

$$ f^\alpha[n(x - a)] = \sum_{q_\perp G} f(q_\perp) e^{i q_\perp \cdot [n(x - a)]} \delta_{q_\perp n, k_\alpha^0 - k_\beta^0 + G}, \quad (3) $$

where $f(q_\perp)$ is a Fourier transformant of $f(nx) = f(x_\perp)$, $f(x_\perp = 0) = f(q_\perp = 0) = 0$.

In the (GaAs)$_n$/(AlAs)$_n$ (001) SL interfaces are located at the distance $na = n(a_0/2)$ from the zero coordinate ($a_0$ is a lattice constant). According to Eq. (3) there are only two perturbation operators that are odd under inversion of $n$ (these operators have different signs for AB/A'B and A'B/AB interfaces), which give a non-zero contribution into $\Gamma-\Gamma$, $X-X$ and $\Gamma-X$ couplings in the first order of the perturbation theory. These operators transform according to respectively $\Gamma_{15}(\Gamma_{15z})$ and $*X_3(X_{3z})$ irreducible representations of the space-group $T_d^2$ (in which $\Delta U(x)$ is invariant)

$$ \hat{V}_{-\alpha}^{(0) \Gamma_{15z}} = \Delta U(x) \sum_{m=1}^{\infty} 2i f \left( \frac{4\pi}{a_0} m \right) \sin \frac{4\pi}{a_0} mz \quad (4) $$

$$ \hat{V}_{-\alpha}^{(0) X_{3z}} = \Delta U(x) \sum_{m=0}^{\infty} 2i f \left[ \frac{2\pi}{a_0} (2m + 1) \right] \sin \frac{2\pi}{a_0} (2m + 1)z \cos \pi (2m + 1)n. \quad (5) $$

Therefore matrix of multiband EMA+SRIC effective Hamiltonian will include only odd under inversion of $n$ corrections of the first order, which have symmetry of $\Gamma_{15} (\Gamma_{15z})$ and $*X_3(X_{3z})$. These corrections lead to $\Gamma_{15x} - \Gamma_{15y}$, $\Gamma_1 - X_{3z}$, $X_{1z} - X_{3z}$ and $X_{3x} - X_{3z}$.
couplings, which fully agrees with [8]. In the framework of a model with limited number of bands, effective Hamiltonian will include corrections of higher orders, which arise due to interactions with other bands. Corrections of even orders are even under inversion of \( n \) and have symmetry of \( \Gamma_1, \Gamma_{12}(\Gamma_{12.1}), \star X_1(X_{1z}) \). Corrections of odd orders are analogous to the corrections of the first order. Even \( \Gamma_1 \) and \( \Gamma_{12}(\Gamma_{12.1}) \) corrections are diagonal, but \( \star X_1(X_{1z}) \) corrections are off-diagonal and lead to \( \Gamma_1 - X_{1z} \) and \( X_{1x} - X_{1y} \) couplings.

2. Electronic structure of \((\text{GaAs})_n/(\text{AlAs})_n\) SL

EMA+SRIC method was used to calculate energy structure of electrons \((\Gamma_1 \oplus \star X_1 \oplus \star X_3 \text{ model})\) and of holes \((\Gamma_8 \oplus \Gamma_7 \text{ model})\) in \((\text{GaAs})_n/(\text{AlAs})_n\) (001) SL with \( n = 1 \ldots 25 \). Reducing of bulk crystal symmetry \( T_d^2 \) to SL symmetry \( D_{2d}^5 \) leads to a split of energy states split

\[
T_d^2 \rightarrow D_{2d}^5 \quad T_d^2 \rightarrow D_{2d}^5
\]

\[
\Gamma_1 \rightarrow \Gamma_1 \quad \star X_1 \rightarrow \Gamma_1 \oplus \star \vec{M}_1 \oplus \star \vec{M}_2 \text{ (even } n \text{)}
\]

\[
\Gamma_7 \rightarrow \Gamma_7 \quad \star X_3 \rightarrow \Gamma_3 \oplus \star \vec{M}_5 \text{ (even } n \text{)}
\]

\[
\Gamma_8 \rightarrow \Gamma_6 \oplus \Gamma_7 \quad \star X_1 \rightarrow \Gamma_1 \oplus \star \vec{M}_5 \text{ (odd } n \text{)}
\]

\[
\star X_3 \rightarrow \Gamma_1 \oplus \star \vec{M}_1 \oplus \star \vec{M}_2 \text{ (odd } n \text{)}
\]

![Fig. 1](image)

**Fig. 1.** Energy of the two lowest conduction states of \((\text{GaAs})_n/(\text{AlAs})_n\) (001) SL.

Figure 1 shows how energy of the two lowest \( \bar{\Gamma}_1(\Gamma_1) \) and \( \bar{\Gamma}_1(X_{1z}) \) states of the conduction band of the SL, which originate from the \( \Gamma_1 \) and \( \star X_1 \) states of the bulk crystal, depend on the period \( n \). Multiband coupling coefficients (Table 1) were determined from

<table>
<thead>
<tr>
<th>( \alpha - \beta )</th>
<th>Coupling coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Gamma_1 - \Gamma_1 )</td>
<td>-0.452</td>
</tr>
<tr>
<td>( X_{1z} - X_{1z} )</td>
<td>0.051</td>
</tr>
<tr>
<td>( X_{3z} - X_{3z} )</td>
<td>0</td>
</tr>
<tr>
<td>( \Gamma_1 - X_{1z} )</td>
<td>-0.101</td>
</tr>
<tr>
<td>( \Gamma_1 - X_{3z} )</td>
<td>-0.562</td>
</tr>
<tr>
<td>( X_{1z} - X_{3z} )</td>
<td>0.539</td>
</tr>
</tbody>
</table>
the best matching of our results with \( n = 1 \) and \( n = 2 \) with the results of the pseudopotential calculations [4] (dots in Fig. 1). It can be seen that there is an excellent agreement of our results for other periods \( (n = 3 \ldots 20) \) with the results obtained in [4]. This proves equivalency of the two following approaches: EMA+SRIC and empirical pseudopotential models. However the EMA+SRIC method, which we used, is much easier and does not require huge computational efforts.

References