

UNCLASSIFIED

Defense Technical Information Center
Compilation Part Notice

ADP013048

TITLE: Multiband Coupling and Electronic Structure of Short-Period
[GaAs]_n/[AlAs]_n [001] Superlattices

DISTRIBUTION: Approved for public release, distribution unlimited
Availability: Hard copy only.

This paper is part of the following report:

TITLE: Nanostructures: Physics and Technology International Symposium
[8th] Held in St. Petersburg, Russia on June 19-23, 2000 Proceedings

To order the complete compilation report, use: ADA407315

The component part is provided here to allow users access to individually authored sections of proceedings, annals, symposia, etc. However, the component should be considered within the context of the overall compilation report and not as a stand-alone technical report.

The following component part numbers comprise the compilation report:

ADP013002 thru ADP013146

UNCLASSIFIED

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

G. F. Glinskii, V. A. *Lakisov*, A. G. Dolmatov and K. O. Kravchenko
Saint-Petersburg Electrotechnical University, St Petersburg, 197376, Russia

Abstract. It is shown that effective mass approximation together with short range interface corrections can be used to calculate short-period abrupt $(\text{GaAs})_n/(\text{AlAs})_n$ (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 $(\text{GaAs})_n/(\text{AlAs})_n$ (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 Γ_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 $(\text{GaAs})_n/(\text{AlAs})_n$ (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 $\Gamma_{15x} - \Gamma_{15y}$ 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 $\Gamma_1 \oplus *X_1 \oplus *X_3$ 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 $(\text{GaAs})_n/(\text{AlAs})_n$ (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

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

Here $U_{1,2}(\mathbf{x})$ are the crystal potentials on the left and right sides of the interface respectively, which have the same period and symmetry; $f[\mathbf{n}(\mathbf{x} - \mathbf{a})]$ is an odd step-function, modulating periodic potential; \mathbf{n} is a unit vector normal to the interface; \mathbf{a} is Bravias 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

$$H_{ni,mj}^{(s)\alpha\beta}(\mathbf{x}) = \langle \alpha, n, \mathbf{k}_i^0 | f[\mathbf{n}(\mathbf{x} - \mathbf{a})]\Delta U(\mathbf{x}) | \beta, m, \mathbf{k}_j^0 \rangle \delta[\mathbf{n}(\mathbf{x} - \mathbf{a})]. \quad (2)$$

Here $|\alpha, n, \mathbf{k}_i^0\rangle$ and $|\beta, m, \mathbf{k}_j^0\rangle$ are Bloch states, which correspond to \mathbf{k}_i^0 and \mathbf{k}_j^0 points of the Brillouin zone of a virtual $\text{Ga}_{0.5}\text{Al}_{0.5}\text{As}$ crystal; α and β 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 $\Delta U(\mathbf{x})$ 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 $f[\mathbf{n}(\mathbf{x} - \mathbf{a})]$

$$f^s[\mathbf{n}(\mathbf{x} - \mathbf{a})] = \sum_{q_\perp, \mathbf{G}} f(q_\perp) e^{iq_\perp[\mathbf{n}(\mathbf{x} - \mathbf{a})]} \delta_{q_\perp \mathbf{n}, \mathbf{k}_i^0 - \mathbf{k}_j^0 + \mathbf{G}}, \quad (3)$$

where $f(q_\perp)$ is a Fourier transformant of $f(\mathbf{n}\mathbf{x}) = f(x_\perp)$, $f(x_\perp = 0) = f(q_\perp = 0) = 0$.

In the $(\text{GaAs})_n/(\text{AlAs})_n$ (001) SL interfaces are located at the distance $\mathbf{n}\mathbf{a} = n(a_0/2)$ 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 \mathbf{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 $\Delta U(\mathbf{x})$ is invariant)

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

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

Therefore matrix of multiband EMA+SRIC effective Hamiltonian will include only odd under inversion of \mathbf{n} corrections of the first order, which have symmetry of $\Gamma_{15}(\Gamma_{15z})$ and $^*X_3(X_{3z})$. These corrections lead to $\Gamma_{15x}-\Gamma_{15y}$, Γ_1-X_{3z} , $X_{1z}-X_{3z}$ and $X_{3x}-X_{3x}$

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 \mathbf{n} and have symmetry of $\Gamma_1, \Gamma_{12}(\Gamma_{12,1}), *X_1(X_{1z})$. Corrections of odd orders are analogous to the corrections of the first order. Even Γ_1 and $\Gamma_{12}(\Gamma_{12,1})$ corrections are diagonal, but $*X_1(X_{1z})$ corrections are off-diagonal and lead to Γ_1-X_{1z} and $X_{1x}-X_{1y}$ couplings.

2. Electronic structure of (GaAs)_n/(AlAs)_n SL

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

$$\begin{array}{ll}
 T_d^2 \longrightarrow D_{2d}^5 & T_d^2 \longrightarrow D_{2d}^5 \\
 \Gamma_1 \longrightarrow \bar{\Gamma}_1 & *X_1 \longrightarrow \bar{\Gamma}_1 \oplus *M_1 \oplus *M_2 \text{ (even } n) \\
 \Gamma_7 \longrightarrow \bar{\Gamma}_7 & *X_3 \longrightarrow \bar{\Gamma}_3 \oplus *M_5 \text{ (even } n) \\
 \Gamma_8 \longrightarrow \bar{\Gamma}_6 \oplus \bar{\Gamma}_7 & *X_1 \longrightarrow \bar{\Gamma}_3 \oplus *M_5 \text{ (odd } n) \\
 & *X_3 \longrightarrow \bar{\Gamma}_1 \oplus *M_1 \oplus *M_2 \text{ (odd } n)
 \end{array}$$

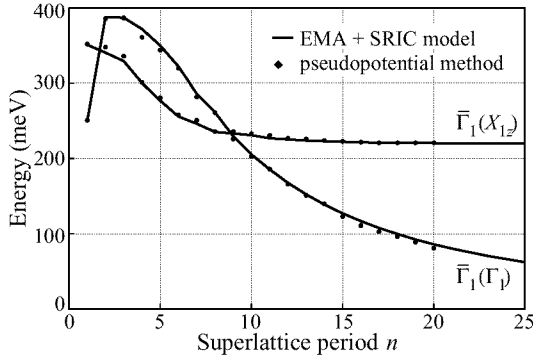


Fig. 1. Energy of the two lowest conduction states of (GaAs)_n/(AlAs)_n (001) SL.

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 Γ_1 and $*X_1$ states of the bulk crystal, depend on the period n . Multiband coupling coefficients (Table 1) were determined from

Table 1. Coupling coefficients (eVÅ) for $\Gamma_1 \oplus *X_1 \oplus *X_3$ model.

$\alpha - \beta$	Coupling coefficients
$\Gamma_1 - \Gamma_1$	-0.452
$X_{1z} - X_{1z}$	0.051
$X_{3z} - X_{3z}$	0
$\Gamma_1 - X_{1z}$	-0.101
$\Gamma_1 - X_{3z}$	-0.562
$X_{1z} - X_{3z}$	0.539

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 ($n = 3 \dots 20$) 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

- [1] D. M. Wood and A. Zunger, *Phys. Rev. B* **53**, 7949 (1996).
- [2] L. W. Wang, A. Franceschetti and A. Zunger, *Phys. Rev. Lett.* **78**, 2819 (1997).
- [3] L. W. Wang and A. Zunger, *Phys. Rev. B* **56**, 12395 (1997).
- [4] L. W. Wang and A. Zunger, *Phys. Rev. B* **59**, 15806 (1999).
- [5] M. G. Burt, *J. Phys. Condens. Matter* **4**, 6651 (1992).
- [6] Y. Fu, M. Willander, E. L. Ivchenko and A. A. Kiselev, *Phys. Rev. B* **47**, 13498 (1993).
- [7] E. L. Ivchenko, A. Yu. Kaminski and U. Rössler, *Phys. Rev. B* **54**, 5852 (1996).
- [8] B. A. Foreman *Phys. Rev. Lett.* **81**, 425 (1998).
- [9] J. G. Menchero, B. Koiller and R. B. Capaz, *Phys. Rev. Lett.* **83**, 2034 (1999).
- [10] H. Im, P. C. Klipstein, R. Grey and G. Hill, *Phys. Rev. Lett.* **83**, 3693 (1999).