Analytical Envelope-Function Theory of Interface Band Mixing

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An analytical theory of intervalley mixing at semiconductor heterojunctions is presented. Burt's envelope-function representation is used to analyze a pseudopotential Hamiltonian, yielding a simple δ-function mixing between Γ and X electrons and light and heavy holes. This coupling exists even for media differing only by a constant band offset (i.e., with *no* difference in Bloch functions). [S0031-9007(98)06534-X]

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It is well known in semiconductor physics that bulk effective-mass theory [1] is not valid at an abrupt heterojunction, since the rapid change in potential at the interface causes a mixing of wave functions in different energy bands, and the neglect of such mixing is a key approximation in the development of this theory. It is consequently almost universally believed that a realistic description of the interface can only be achieved numerically, by performing a microscopic supercell calculation. The purpose of this paper is to demonstrate that a careful application of modern envelope-function theory yields a fully *analytical* description of interface band mixing.

The most widely used form of envelope-function theory is Bastard's "envelope-function approximation" (EFA) [2], which openly ignores any interband mixing not found in bulk $\mathbf{k} \cdot \mathbf{p}$ theory [3]. Less well known is Burt's theory of the envelope-function *representation* [4,5], which is an exact representation of the Schrödinger equation, fully capable of describing any effect found in pseudopotential theory. Thus far, the main applications of this theory have been a one-dimensional proof [5] that in long-period superlattices, interface-induced mixing is a small perturbation on the EFA, and the resolution of an ambiguity in the EFA ordering of differential operators [6,7].

Unfortunately, the former work [5] is often misconstrued as implying that Burt's theory is no different from the EFA [8–11]. This interpretation is not warranted, because even small perturbations can have a dramatic impact when they introduce couplings of a qualitatively different nature. In this paper the envelope-function representation is used to analyze an empirical pseudopotential model [12] of the GaAs/AlAs (001) heterojunction. The result is a simple analytical theory of the interface-induced mixing between Γ and X electrons [13–16] and light and heavy holes [17–19], in which the coupling takes the form of a finite-width δ function whose strength is given directly in terms of pseudopotential form factors. The most striking outcome is that there is *no* limit in which the EFA is valid for abrupt heterojunctions, since the coupling exists even for *identical* Bloch functions.

I begin by presenting a paraphrased (nonrigorous) version of Burt's theory. Let the microscopic Hamiltonian be $H = p^2/2m + V(\mathbf{r})$, and choose as basis functions the complete orthonormal Luttinger-Kohn functions [1] $\chi_n(\mathbf{r}) = U_n(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$, where $U_n(\mathbf{r})$ is a periodic Bloch function from some bulk reference crystal (e.g., the virtual crystal $\mathrm{Al_{0.5}Ga_{0.5}As}$). The U_n need not come from Γ, since Bloch functions from X and L are periodic if one adopts a nonprimitive unit cell (e.g., a simple cubic lattice with an 8-atom basis for X, or an fcc lattice with a 16-atom basis for both L and X), which effectively folds these points onto Γ.

To form an envelope-function Hamiltonian $H_{nn'}(\mathbf{r})$, the first step is to sandwich H between two basis states:

$$\chi_n^* H \chi_{n'} = U_n^* \left(H + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m} \right) U_{n'}, \quad (1)$$

thus generating the familiar $\mathbf{k} \cdot \mathbf{p}$ perturbations [3]. The second step is to send (1) through a low-pass filter, removing all Fourier components outside the Brillouin zone. This step is an integral part of the change of representation; it does *not* result in loss of information [4,5]. It is roughly equivalent to averaging (1) over a unit cell [20], so for simplicity the latter procedure will be adopted here. This yields

$$H_{nn'}(\mathbf{r}) = [U_n|H|U_{n'}] + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p}_{nn'} + \frac{\hbar^2 k^2}{2m} \delta_{nn'}, \quad (2)$$

where the brackets [ ] denote an average over a unit cell centered on $\mathbf{r}$, and $\mathbf{p}_{nn'} = [U_n|\mathbf{p}|U_{n'}]$ is independent of $\mathbf{r}$. The final step is to let $\mathbf{k} = -i\nabla$, in which case (2) is just the local version of Burt's Hamiltonian [4,5].

The primary difference between (2) and the EFA Hamiltonian is that (2) does not exclude the interface region from the averaging process. To apply (2), one needs explicit basis functions U_n for zinc-blende semiconductors. In the pseudopotential method [12], one expands these functions in a small number of plane waves,

$$U_n(\mathbf{r}) = \sum_{\mathbf{G}} U_{n\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}, \quad (3)$$

where $\mathbf{G}$ is a reciprocal-lattice vector. In GaAs and AlAs, the states n of interest have symmetry Γ_1, Γ_{15}, X_1, and X_3 [12]. One can use group-theory projection operators [21,22] to symmetrize expansion (3) for each of these representations in turn. This reduces (3) to the form

$$U_n(\mathbf{r}) = \sum_i C_n^i U_n^i(\mathbf{r}), \quad (4)$$

where the coefficients C_n^i satisfy $\sum_i |C_n^i|^2 = 1$, and the functions $U_n^i(\mathbf{r})$ are given in Table I (for states with kinetic energy up to 2 Ry) and Ref. [23] (up to 5 Ry). The origin of coordinates is fixed at an anion site, with a neighboring cation at $\frac{1}{4}a[111]$ (where a is the cubic lattice parameter). The index i refers to the value of G^2 in units of $(2\pi/a)^2$, with an additional label a or c referring in a rough sense to whether a state is centered on the anion or cation. For the triply degenerate Γ_{15}, X_1, and X_3 representations, only the z state is listed; x and y states are given by cyclic permutations.

The coefficients C_n^i are found by diagonalizing H in a bulk crystal, where the pseudopotential takes the form

$$\begin{aligned} V_b = {} & V_0^S + 4V_3^a U_{\Gamma_1}^{3a}/\sqrt{8} \\ & + 4V_3^c U_{\Gamma_1}^{3c}/\sqrt{8} - 2V_4^A U_{\Gamma_1}^{4}/\sqrt{2/3} \\ & + 4V_8^S U_{\Gamma_1}^{8}/\sqrt{4/3} + 4V_{11}^a U_{\Gamma_1}^{11a}/\sqrt{8/3} \\ & - 4V_{11}^c U_{\Gamma_1}^{11c}/\sqrt{8/3} - 8V_{12}^A U_{\Gamma_1}^{12A}/\sqrt{8} . \end{aligned} \tag{5}$$

Here the expansion coefficients are standard pseudopotential form factors [12], with $V_3^a = V_3^S - V_3^A$ and $V_3^c = V_3^S + V_3^A$. The Bloch functions of interest are tabulated in Ref. [23], using the phase convention $U_n(\mathbf{0}) > 0$ for Γ_1 and X_1, and $\partial U_n(\mathbf{0})/\partial z > 0$ for Γ_{15z} and X_{3z}.

The Bloch functions of GaAs and AlAs are very similar, so their differences can be treated accurately in perturbation theory [24]. Since Bloch functions cannot be identical unless the bulk potentials (5) are identical (to within a constant offset ΔV_0^S), the actual perturbation is the difference between the heterostructure potential $V(\mathbf{r})$ and the reference ($Al_{0.5}Ga_{0.5}As$) potential. The present work considers only first-order interface effects—namely, the direct matrix elements of $V(\mathbf{r})$ within the manifold consisting of the ground Γ_{15} and first excited Γ_1, X_1, and X_3 states of the reference crystal. Second-order effects are also of some importance, but their analysis will be deferred to a later, more extensive publication.

To illustrate the techniques involved, the coupling between the Γ_{15x} and Γ_{15y} valence bands is calculated in detail below. The simplest model of a heterojunction is an abrupt planar junction, in which each form factor in (5) has a step discontinuity at the interface (namely, the As plane $z = 0$). Consider first the $G = 0$ form factor $V_0^S(z)$. Averaging over the xy plane, one finds

$$[U_{\Gamma_{15x}}|V_0^S|U_{\Gamma_{15y}}]_{xy} = 2C_{\Gamma_{15}}^{3a}C_{\Gamma_{15}}^{3c}V_0^S(z)\sin(4\pi z/a) . \tag{6}$$

The average of this function between $z - \frac{1}{4}a$ and $z + \frac{1}{4}a$ is zero when $|z| > \frac{1}{4}a$, since $V_0^S(z)$ is constant apart from a step of ΔV_0^S at $z = 0$. Thus, as expected, there is no zone-center Γ_{15x}-Γ_{15y} coupling in bulk material. However, in the interface region $|z| < \frac{1}{4}a$, the average is no longer zero:

$$[U_{\Gamma_{15x}}|V_0^S|U_{\Gamma_{15y}}] = \frac{1}{\pi} C_{\Gamma_{15}}^{3a}C_{\Gamma_{15}}^{3c}\Delta V_0^S(1 + \cos 4\pi z/a) . \tag{7}$$

This is a δ-like function of width $\frac{1}{2}a$. Since slowly varying envelope functions are primarily sensitive to the area under this function, one can replace (7) for most purposes by a coupling of the form $\Omega_{nn'}\delta(z)$, where

$$\Omega_{\Gamma_{15x}\Gamma_{15y}} = \frac{a}{2\pi} C_{\Gamma_{15}}^{3a}C_{\Gamma_{15}}^{3c}\Delta V_0^S . \tag{8}$$

This seemingly trivial result has important consequences. First, the use of δ-function coupling in phenomenological theories of intervalley mixing [13,15–19] has been given a simple and direct justification. Second, this coupling exists even when the Bloch functions of two media are *exactly* the same (since a constant offset ΔV_0^S has no effect on the Bloch functions). Hence there is *no* limit in which the EFA is valid at an abrupt heterojunction.

One can now apply the same averaging process to each of the remaining terms in (5). The resulting coefficient $\Omega_{nn'}$ is conveniently expressed in the form

$$\Omega_{nn'} = \frac{a}{4\pi} \sum_{i,j} C_n^i (P_{ij} + W_{ij}) C_{n'}^j , \tag{9}$$

where the matrix P_{ij} is given in Table II for Γ_{15x}-Γ_{15y} coupling (see Ref. [23] for other types of coupling), and W_{ij} is discussed below. Using the 5-Ry Bloch functions of $Al_{0.5}Ga_{0.5}As$ tabulated in [23], one finds

$$\begin{aligned} \Omega_{\Gamma_{15x}\Gamma_{15y}} = \frac{a}{2\pi} [& 0.35\Delta V_0^S + 0.40\Delta V_3^a + 0.41\Delta V_3^c \\ & - 0.28\Delta V_4^A - 0.16\Delta V_8^S - 0.42\Delta V_{11}^a \\ & - 1.16\Delta V_{11}^c + 0.13\Delta V_{12}^A] . \end{aligned} \tag{10}$$

The numerical coefficients in (10) were calculated using the pseudopotentials of Ref. [15], but they do not change much if other pseudopotentials (e.g., [25,26]) are used instead. The main variation comes from the explicit form-factor dependence shown in (10).

TABLE I. Γ and X basis functions for a kinetic-energy cutoff of 2 Ry (given in units where $2\pi/a = 1$).

i	$U_{\Gamma_i}^i(\mathrm{r})$	$U_{\Gamma_{15z}}^i(\mathrm{r})$	j	$U_{X_{1z}}^j(\mathrm{r})$	$U_{X_{3z}}^j(\mathrm{r})$
0	1	$\cdots$	1	$\sqrt{2}\cos z$	$\sqrt{2}\sin z$
$3a$	$\sqrt{8}\cos x\cos y\cos z$	$\sqrt{8}\cos x\cos y\sin z$	2	$2\cos x\cos y$	$2\sin x\sin y$
$3c$	$\sqrt{8}\sin x\sin y\sin z$	$\sqrt{8}\sin x\sin y\cos z$	5	$\sqrt{2}(\cos 2x + \cos 2y)\cos z$	$\sqrt{2}(\cos 2x + \cos 2y)\sin z$
4	$\sqrt{2/3}(\cos 2x + \cos 2y + \cos 2z)$	$\sqrt{2}\sin 2z$			

TABLE II. Interface coefficients $P_{ij} = P_{ji}$ for coupling between Γ_{15x} and Γ_{15y} at a planar interface.

$i\backslash j$	$3a$	$3c$	4
$3a$	0	$\Delta V_0^S - \frac{1}{2}\Delta V_4^A - \Delta V_8^S + \frac{1}{2}\Delta V_{12}^A$	$\Delta V_3^c - \frac{5}{2}\Delta V_{11}^c$
$3c$		0	$\Delta V_3^a - \frac{3}{2}\Delta V_{11}^a$
4			0

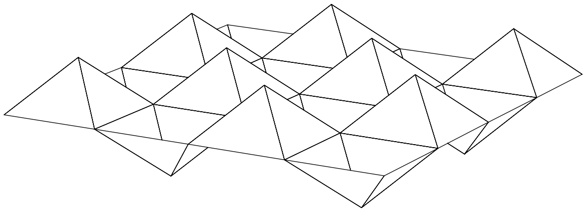

FIG. 1. Surface separating the two bulk regions of a (001) AlAs/GaAs heterojunction in the waffle interface model.

At this stage, one may wonder how much the result (10) depends on the initial assumption of a planar interface. This question will be addressed by modifying the potential to include information about the atomic structure of the interface [27]. The potential will still be piecewise periodic, but its value at any given point will now be determined by the cation and anion closest to that point. If these are Ga and As, the potential is that of bulk GaAs; if they are Al and As, it is that of bulk AlAs. This is equivalent to constructing fcc Wigner-Seitz cells around each cation and anion, and defining the potential by the regions of overlap between cells. Such a model should provide a reasonable first approximation to the effects of charge transfer at a real heterojunction [27].

Within this model the interface has the "waffle" shape shown in Fig. 1, in which the influence of atoms near the interface extends a distance $\frac{1}{4}a$ beyond the plane $z = 0$. For example, at an AlAs/GaAs (001) junction, the Al atom at $\frac{1}{4}a[\bar{1}1\bar{1}]$ may lie below $z = 0$, but it still governs the potential for $0 < z < \frac{1}{4}a$ over a region of square cross section given by $(z - \frac{1}{2}a < x < -z, z < y < -z + \frac{1}{2}a)$. Similarly, the Ga atom at $\frac{1}{4}a[111]$ governs the potential for $-\frac{1}{4}a < z < 0$ over the region $(-z < x < z + \frac{1}{2}a, -z < y < z + \frac{1}{2}a)$. One can treat this "waffling" as a perturbation on the planar interface and calculate its contribution to $\Omega_{nn'}$ just as before; this is the source of the extra term W_{ij} in Eq. (9). The matrix W_{ij} is given in Ref. [23]; its effect is to change $\Omega_{\Gamma_{15x}\Gamma_{15y}}$ from (10) to

$$\Omega_{\Gamma_{15x}\Gamma_{15y}} = \frac{a}{2\pi}[0.69\Delta V_0^S + 0.94\Delta V_3^a + 0.25\Delta V_3^c - 0.76\Delta V_4^A - 0.21\Delta V_8^S - 0.73\Delta V_{11}^a - 0.64\Delta V_{11}^c + 0.14\Delta V_{12}^A]. \tag{11}$$

Obviously the deviations from planarity are not negligible, since many of the coefficients have changed by a factor of 2 or more.

A final source of concern is the discontinuous nature of the junction potential; such a potential clearly cannot be self-consistent. A simple way to compensate for this may be obtained by examining the effects of self-consistency in the screening of an external charge by an electron gas. An external charge $\rho_{\text{ext}}(\mathbf{r})$ placed in an electron gas will attract an induced charge $\rho_{\text{ind}}(\mathbf{r})$; in linear-response theory, this effect is described in Fourier space by the dielectric function $\epsilon(\mathbf{q}) = \rho_{\text{ext}}(\mathbf{q})/[\rho_{\text{ext}}(\mathbf{q}) + \rho_{\text{ind}}(\mathbf{q})]$. If there were no such thing as the uncertainty principle or electron-electron interactions, screening would be *perfect*: an external charge $\rho_{\text{ext}}(\mathbf{r}) = e\delta(\mathbf{r})$ would generate a response $\rho_{\text{ind}}(\mathbf{r}) = -e\delta(\mathbf{r})$, i.e., $\epsilon(\mathbf{q}) = \infty$.

Such a sharply peaked response is, of course, physically inadmissible; uncertainty and electron-electron interactions tend to smooth the response, with the result that screening is never absolute. This smoothing effect is characterized by the function $S(\mathbf{q}) = -\rho_{\text{ind}}(\mathbf{q})/\rho_{\text{ext}}(\mathbf{q}) = 1 - \epsilon^{-1}(\mathbf{q})$. For perfect screening, one has $S(\mathbf{q}) = 1$, but for Thomas-Fermi screening, the large-q components are filtered out: $S(\mathbf{q}) = (1 + q^2/k_s^2)^{-1}$, where k_s^{-1} is the screening length (which is about $\frac{1}{5}$ of the nearest-neighbor spacing in GaAs). The function $S(\mathbf{q})$ will be used here to smooth the transition between bulk potentials. For simplicity, $\epsilon(\mathbf{q})$ is taken to be the Lindhard dielectric function of a free-electron gas with a density of eight valence electrons per primitive unit cell.

Smoothing is easier to apply in the plane-wave basis (3) than in the symmetrized basis (4). Indeed, in a plane-wave basis, one can use the same expression for all types of interband mixing:

$$\Omega_{nn'} = \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}''} U_{n\mathbf{G}}^* U_{n'\mathbf{G}'} \Delta V_{\mathbf{G}''} I(\mathbf{G} - \mathbf{G}' - \mathbf{G}''). \tag{12}$$

Here $I(\mathbf{G})$ is just the Fourier transform of the interface function; e.g., for a smoothed planar interface, it is the transform of a unit step function multiplied by $S(\mathbf{G})$:

$$I(\mathbf{G}) = \delta_{G_x,0}\,\delta_{G_y,0}(1 - \delta_{G_z,0})\frac{1}{iG_z}S(\mathbf{G}). \tag{13}$$

This was used in [4,5] (with $S = 1$) to study Γ electron-hole mixing in one dimension. For the waffle interface,

$$\begin{aligned} I(\mathbf{G}) = (1 - \delta_{\mathbf{G},\mathbf{0}})\Big\{&(1 - \delta_{G_y,0})\frac{i}{4G_y}[e^{iG_x a/4}\operatorname{sinc}(\mathbf{G}\cdot\tau_0)\operatorname{sinc}(\mathbf{G}\cdot\tau_1) - e^{-iG_x a/4}\operatorname{sinc}(\mathbf{G}\cdot\tau_2)\operatorname{sinc}(\mathbf{G}\cdot\tau_3)] \\ &+ \delta_{G_y,0}\frac{G_z}{i(G_x \mp G_z)^2}\operatorname{sinc}^2[(G_x \pm G_z)a/8]\Big\}S(\mathbf{G}), \end{aligned} \tag{14}$$

TABLE III. Coupling coefficients $\Omega_{nn'}$ (eV Å) at an AlAs/GaAs (001) "smooth waffle" interface [Eq. (14)], with a kinetic-energy cutoff of 5 Ry.

	Source of psuedopotential			
n-n'	Ref. [15]	Ref. [25]	Ref. [26]	Ref. [28]
Γ_{15x}-Γ_{15y}	0.19	0.11	0.14	0.31
Γ_1-Γ_{15z}	−0.01	−0.08	−0.19	0.02
Γ_1-X_{3z}	−0.21	−0.29	−0.07	−0.67
X_{1z}-X_{3z}	0.11	0.01	0.21	0.25
X_{3x}-X_{3y}	−0.34	−0.30	0.05	−0.54

where $\mathrm{sinc}(x) = \sin(x)/x$, $\boldsymbol{\tau}_0 = \frac{1}{8}a[111]$, $\boldsymbol{\tau}_1 = \frac{1}{8}a[1\bar{1}\bar{1}]$, $\boldsymbol{\tau}_2 = \frac{1}{8}a[\bar{1}1\bar{1}]$, and $\boldsymbol{\tau}_3 = \frac{1}{8}a[\bar{1}\bar{1}1]$. The $\pm$ signs in (14) are used to avoid a possible divergence at $G_x = \pm G_z$.

Smoothing tends to reduce the magnitude of $\Omega_{nn'}$. For example, for the pseudopotentials of Ref. [15], $\Omega_{\Gamma_{15x}\Gamma_{15y}}$ is 0.082 eV Å for an abrupt planar interface, 0.056 eV Å for a smooth planar interface, 0.30 eV Å for an abrupt waffle interface, and 0.19 eV Å for a smooth waffle interface. Hence the choice of model has a significant impact on the strength (and sign) of the interface coupling.

The choice of pseudopotential is also significant. Table III compares various empirical pseudopotentials for different types of coupling between Γ and X states. No critical evaluation of these potentials is attempted here (see [28]); the purpose of this table is merely to emphasize that the envelope-function representation permits one to ascertain in detail how a given choice of pseudopotential influences the intervalley coupling.

The coupling coefficients derived here provide a direct link between microscopic theory and recent phenomenological models of valence-band [17–19] and Γ-X [13,15,16] mixing. Such models have proven capable of reproducing experimentally measured mixing effects in all but the shortest-period superlattices. The values in Table III are similar to the estimates used in these papers; however, in contrast with Ref. [16], the present work gives $\Omega_{X_{1x}X_{1y}} = 0$ [29] and $\Omega_{X_{1z}X_{3z}} \neq 0$.

Spin-orbit coupling was omitted here because it is generated almost entirely in the atomic cores [3], with the outer electrons contributing very little, even at an abrupt junction. Therefore, it need not be introduced until *after* the interface coupling has been calculated. In a spin-dependent theory, Γ_{15x}-Γ_{15y} mixing leads to a mixing between Γ_8 light and heavy holes [17–19].

Several other methods have been proposed for incorporating interface mixing into $\mathbf{k}\cdot\mathbf{p}$ theory [14,24,30–32]. Like the present work, they sharply reduce the computational cost of realistic band-structure calculations. However, these models are all essentially numerical in character; none of them provides the simple, direct picture of the interface physics that is offered by the envelope-function representation.

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