Tunneling and propagating transport in GaAs–Ga$_{1-x}$Al$_x$As–GaAs(100) double heterojunctions[a)]

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We present a study of the transport characteristics of electrons through abrupt GaAs–Ga$_{1-x}$Al$_x$As–GaAs(100) double heterojunctions. The theoretical apparatus uses complex-**k**-band structures in the tight-binding approximation and transfer matrices. States on each side of the Ga$_{1-x}$Al$_x$As central barrier are expanded in terms of a complex-**k**-bulk state basis so as to provide a description of the wave function at the GaAs–Ga$_{1-x}$Al$_x$As(100) interface. We treat the case where the incoming state in GaAs is derived from near the conduction band Γ point. Transmission through the Ga$_{1-x}$Al$_x$As barrier is either tunneling or propagating depending on the nature of the Bloch states available for strong coupling in the alloy. States derived from the same extremum of the conduction band appear to couple strongly to each other across the GaAs–Ga$_{1-x}$Al$_x$As interface. Transport characteristics of incoming states derived from near the conduction band Γ point are examined as a function of the energy of the incoming state, thickness of the Ga$_{1-x}$Al$_x$As barrier, and alloy composition x. Transmission through the Ga$_{1-x}$Al$_x$As barrier is either tunneling or propagating, depending on the nature of the Bloch states available for strong coupling in the alloy.

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I. INTRODUCTION

The introduction of new device fabrication technologies has allowed the realization of planar electronic devices in which the dimension perpendicular to the growth plane is of the order of a few lattice spacings. The understanding of electron states at semiconductor interfaces is of great importance regarding the performance of these very small-scale electronic devices. The work presented here is concerned with the transport of electrons through a GaAs–Ga$_{1-x}$Al$_x$As-GaAs(100) double heterojunction structure (DHS).

The mode of transport in these structures is either *tunneling* (energy less than the potential barrier height) or *propagating* (energy greater than the potential barrier height). In the former, the Bloch states available for transmission in the Ga$_{1-x}$Al$_x$As are *evanescent* and the wave vector **k** is complex. In the latter, the Bloch states available for transmission in the alloy are *propagating* and the wave vector **k** takes on real values.

The theoretical framework exploits the bulk properties of the constituent semiconductors forming the DHS. The transport of electrons through a region of space in which the energy of the electron is such that free propagation is not allowed is best described in terms of the complex-**k**-bulk band structure. The breakdown of translational invariance induced by the interface implies a new set of boundary conditions that do not exclude the component of the wave vector **k** normal to the interface to take on complex values. The bulk Bloch states associated with complex **k** provide then a suitable basis for a full description of the wave function. The problem of calculating the transport coefficients of Bloch states at an abrupt interface using complex-**k**-band structure, cast in a tight-binding band calculation scheme, has been addressed in the past.[1–4] It is only recently that an expedient method, applicable to tight-binding, pseudopotential, and **k·p** band calculation formalisms, has been devised to reduce the problem of calculating the complex-**k**-band structure to that of an associated eigenvalue problem.[5,6]

The paper is organized as follows: In Sec. II, the basic ingredients of the technique used to calculate the transport coefficients are presented. The major results are discussed in Sec. III. A summary and conclusions are given in Sec. IV.

II. CALCULATIONAL METHOD

The system studied consists of a barrier of Ga$_{1-x}$Al$_x$As located between two semi-infinite layers of GaAs. Figure 1 illustrates the system studied. An electron incoming from bulk region I (GaAs) at an energy E, above the GaAs conduction band minimum, is scattered at the boundaries of the barrier region II (Ga$_{1-x}$Al$_x$As) and is finally transmitted in another bulk region III (GaAs). The Γ-point conduction band potential barrier at the interface, ΔE_Γ, is taken to be a fraction of the difference in the Γ-point band gaps between GaAs and Ga$_{1-x}$Al$_x$As. Depending on whether we describe the total wave function in a bulk region or a barrier region, different representations are used accordingly. We now discuss these two representations.

Systems which exhibit two-dimensional periodicity are best described in a planar orbital representation.[7–10] A planar orbital is a two-dimensional Bloch sum consisting of localized atomic functions. Let $\hat{\mathbf{z}}$ be the direction normal to the interface and $\mathbf{k}_\parallel = \hat{\mathbf{x}}k_x + \hat{\mathbf{y}}k_y$ be the two-dimensional

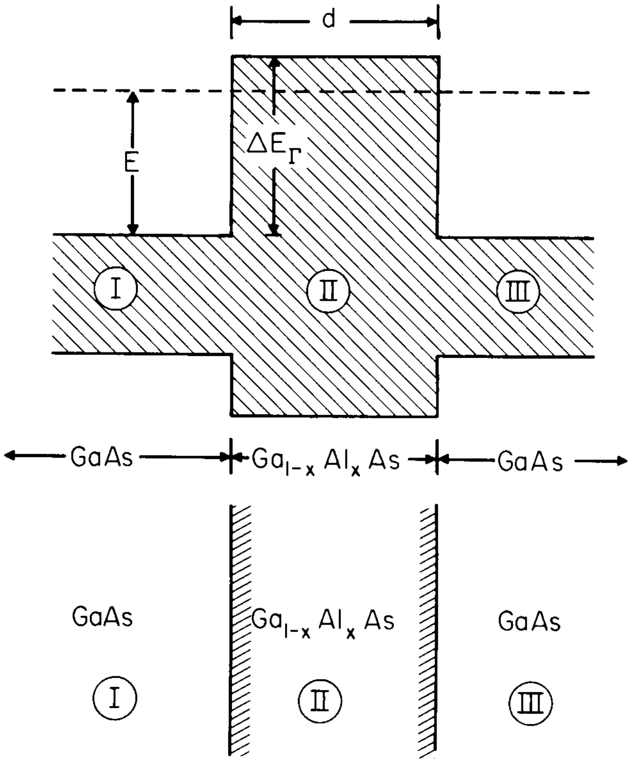

FIG. 1. Energy band diagram of GaAs–$Ga_{1-x}Al_xAs$–GaAs DHS and corresponding physical structure. The electron is derived from the GaAs Γ point and has a total energy E measured with respect to the GaAs Γ-point conduction band minimum. The Γ-point conduction band offset is indicated by ΔE_Γ. The thickness of the $Ga_{1-x}Al_xAs$ barrier is d.

wave vector parallel to the interface. Let $\phi_\alpha(\mathbf{k}_\parallel;\sigma)$ designate the planar orbital corresponding to a given atomic orbital type α within the layer σ. The Bloch states $\psi(\mathbf{k}_\parallel,k_z)$, labeled by the wave vector $\mathbf{k} = \mathbf{k}_\parallel + \hat{\mathbf{z}}k_z$, are expanded in terms of this set of planar orbitals $\{\phi_\alpha(\mathbf{k}_\parallel;\sigma)\}$. For interface systems, k_z is complex in general.

Where the total Hamiltonian is bulklike, the wave function is expanded in a set of bulk Bloch states $\{\psi(\mathbf{k}_\parallel,k_z)\}$. On each sides of an interface connecting two bulklike regions, the wave function is described in a planar orbital representation $\{\phi_\alpha(\mathbf{k}_\parallel;\sigma)\}$, and transfered across the interface using a transfer matrix. The connection between the bulk Bloch states representation $\{\psi(\mathbf{k}_\parallel,k_z)\}$ and the planar orbital representation, $\{\phi_\alpha(\mathbf{k}_\parallel;\sigma)\}$ is described in Ref. 6 and will not be repeated here.

The total number N of Bloch states $\psi(\mathbf{k}_\parallel,k_\lambda)$ with $k_z = k_\lambda$ ($\lambda = 1,\ldots,N$) corresponding to a given parallel wave vector $\mathbf{k}_\parallel$ and energy E depends on the particular tight-binding model used and on the orientation of the interface plane. More specifically, the total number of Bloch states $\psi(\mathbf{k}_\parallel,k_\lambda)$ with real or complex wave vector k_λ is equal to the product of the number of atomic orbitals per atom times the number of layers interacting with a given layer.[1] In the tight-binding representation used here, we have five orbitals per atom (s^*,s,p_x,p_y,p_z)[11] and only first nearest-neighbor interactions were included. There are, therefore, ten Bloch states ($N = 10$) for each parallel wave vector $\mathbf{k}_\parallel$ and total energy E. Half of the states have to be discarded because they either grow away from the interface, if $\mathrm{Im}(k_z)$ does not have the proper sign, or are propagating in the wrong direction when k_z is real.

Let the incoming Bloch state $\psi(\mathbf{k}_\parallel,k_0)$ with real wave vector k_0 be incident from the left in GaAs onto the GaAs–$Ga_{1-x}Al_xAs$ interface. The total wave function on a given layer σ can be written as[1]

$$\Psi(\mathbf{k}_\parallel,E;\sigma) = \psi(\mathbf{k}_\parallel,k_0;\sigma) + \sum_{k_\lambda} A^{(I)}_{k_\lambda}(\mathbf{k}_\parallel,E)\psi(k_\parallel,k_\lambda;\sigma), \text{ in region } I, \tag{1a}$$

$$\Psi(\mathbf{k}_\parallel,E;\sigma) = \sum_{\alpha} B^{(II)}_{\alpha}(\mathbf{k}_\parallel,E,\sigma)\phi_\alpha(\mathbf{k}_\parallel;\sigma), \text{ in region II}, \tag{1b}$$

$$\Psi(\mathbf{k}_\parallel,E;\sigma) = \sum_{k_\lambda} A^{(III)}_{k_\lambda}(\mathbf{k}_\parallel,E)\psi(k_\parallel,k_\lambda;\sigma), \text{ in region III}. \tag{1c}$$

At fixed energy E and parallel wave vector $\mathbf{k}_\parallel$, we denote by $R_\lambda(\mathbf{k}_\parallel,E)$ and $T_\lambda(\mathbf{k}_\parallel,E)$ the k_z-resolved reflection and transmission coefficients corresponding to the Bloch state $\psi(\mathbf{k}_\parallel,k_\lambda)$. The total transport coefficients $R(\mathbf{k}_\parallel,E)$ and $T(\mathbf{k}_\parallel,E)$ are just the sum of the transport coefficients $R_\lambda(\mathbf{k}_\parallel,E)$ and $T_\lambda(\mathbf{k}_\parallel,E)$. Flux conservation requires $R(\mathbf{k}_\parallel,E) + T(\mathbf{k}_\parallel,E) = 1$.

As shown in Ref. 1, the transmission coefficient for the Bloch state $\psi(\mathbf{k}_\parallel,k_\lambda)$ vanishes when the wave vector of the incoming Bloch state k_0 approaches a critical point such that $[\partial E(\mathbf{k})/\partial k_z]_{k_z=k_0} = 0$. In that case, the incoming state is identical with the reflected state. At this critical point, the incoming state $\psi(\mathbf{k}_\parallel,k_0)$ carries no momentum across the interface and does not couple to any Bloch states in $Ga_{1-x}Al_xAs$. Therefore, transmission starts to occur as the incident wave vector k_0 moves away from the critical point.

The transport states originate in the complex-**k**-band structure of GaAs and $Ga_{1-x}Al_xAs$. The complex-**k**-band structure for GaAs and AlAs is well known.[1,12] We have used similar techniques to obtain the complex-**k**-band structure for $Ga_{1-x}Al_xAs$ within the virtual crystal approximation. Within the ten-band tight-binding description used here, the GaAs Γ-point conduction band minimum is at an energy $E_\Gamma^{\mathrm{GaAs}} \approx 1.51$ eV above the GaAs Γ-point valence band maximum, and the GaAs X-point conduction band valley is at an energy $E_X^{\mathrm{GaAs}} \approx 0.52$ eV above the GaAs Γ-point conduction band minimum.

We denote the bulk states with $k_z = k_\lambda$ in spatial region μ by $\psi(\mathbf{k}_\parallel,k_\lambda^\mu)$. In the discussion that follows, the incident Bloch state is derived from near the GaAs conduction band Γ point with real wave vector $k_0 \equiv k_\Gamma^I$, e.g., $\psi(\mathbf{k}_\parallel,k_0) \equiv \psi(\mathbf{k}_\parallel,k_\Gamma^I)$. The k_z values of interest are those near the conduction band extrema $\Gamma(k_\Gamma)$ and $X(k_X)$. In the energy range between the bottom of the GaAs conduction band and the GaAs X-point valley, k_Γ^I is real and k_X^I is complex such that $\psi(\mathbf{k}_\parallel,k_\Gamma^I)$ has a traveling character and $\psi(\mathbf{k}_\parallel,k_X^I)$ has an evanescent character. However, in the energy range above the X-point valley, both k_Γ^I and k_X^I are real such that $\psi(\mathbf{k}_\parallel,k_\Gamma^I)$ and $\psi(\mathbf{k}_\parallel,k_X^I)$ have traveling character. Similar considerations apply to the Bloch states available for transport in the alloy $Ga_{1-x}Al_xAs$.

For an alloy composition $x < 0.45$,[13] $Ga_{1-x}Al_xAs$ is direct and $E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} < E_X^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$ in this composition range. Throughout the calculations, the conduction band offset ΔE_Γ was taken to be equal to 85% of the difference of Γ-point band gaps between GaAs and $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$.[13,14] The dependence on the alloy composition x of the Γ-point energy edge in $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is, in the virtual crystal approximation: $E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} \approx 1.35x$ eV, above the GaAs Γ-point conduction band minimum.

III. RESULTS

We present the main results for the transmission coefficients of electrons through a GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$–GaAs DHS. The incident Bloch state is derived from near the GaAs conduction band Γ point with real wave vector $k_0 \equiv k_\Gamma^I$, e.g., $\psi(\mathbf{k}_\parallel, k_0) \equiv \psi(\mathbf{k}_\parallel, k_\Gamma^I)$. We discuss the transport across the central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier as a function of the energy E, of the incoming Bloch state $\psi(\mathbf{k}_\parallel, k_0)$, thickness of the barrier and alloy composition x in the central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier.

A. Qualitative features of transport

Figure 2 shows the total transmission and reflection coefficients $T(\mathbf{k}_\parallel, E)$ and $R(\mathbf{k}_\parallel, E)$ as a function of the energy E of the incoming Bloch state. Energy is measured with respect to the GaAs conduction band minimum. We consider the case of vanishing parallel wave vector $\mathbf{k}_\parallel = 0$ and composition of $x = 1.0$. Calculations were carried out for different AlAs barrier thicknesses.

For energies of the incoming states near the GaAs conduction band Γ point, transmission through the AlAs barrier occurs mostly via the coupling to evanescent states that connect to the AlAs conduction band at the Γ point. In the energy range considered, no propagating Bloch states are available in AlAs and the wave function has an evanescent character in the barrier. The AlAs Γ-point minimum is at an energy $E_\Gamma^{\mathrm{AlAs}} = 1.35$ eV above the GaAs conduction band minimum. As mentioned in Sec. II, the transmission coefficient vanishes for incoming states derived from near the conduction band Γ point at an energy equal to E_Γ^{GaAs}. At this energy, the component of the group velocity normal to the interface vanishes $[\partial E(\mathbf{k})/\partial k_z]_{k_z = k_\Gamma^I} \equiv 0$, and the incoming state $\psi(\mathbf{k}_\parallel, k_\Gamma^I)$ does not couple to any states in AlAs.

We now examine the different transport regimes. Figure 3 shows the total transmission coefficient $T(\mathbf{k}_\parallel, E)$ as a function of the number of monolayers forming the central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier. Layers are measured in units of $a/2$, where a is the GaAs lattice constant. Energies of the incoming Bloch state $\psi(\mathbf{k}_\parallel, k_\Gamma^I)$ range from $0.19 \text{ eV} \leqslant E \leqslant 0.69$ eV, measured with respect to the GaAs conduction band minimum. The alloy composition is $x = 0.3$ and $\mathbf{k}_\parallel = 0$. The alloy is direct and the Γ-point energy edge of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is

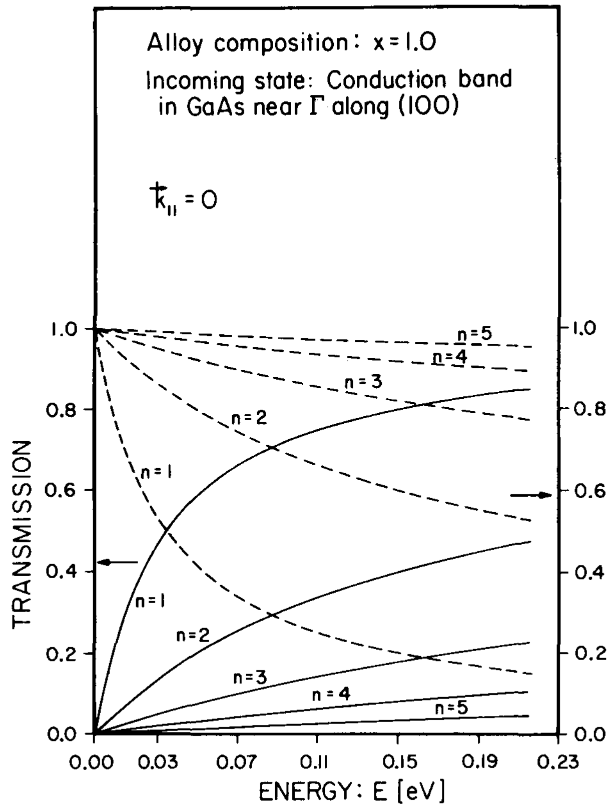

FIG. 2. Total transmission (solid line) and reflection (dashed line) coefficients $T(\mathbf{k}_\parallel, E)$ and $R(\mathbf{k}_\parallel, E)$ as a function of the energy E of the incident Bloch state $\psi(\mathbf{k}_\parallel, k_\Gamma)$ for different $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier thicknesses with an alloy composition of $x = 1.0$. Energy is measured with respect to the GaAs conduction band minimum and $\mathbf{k}_\parallel = 0$. The number of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier layers is n. Incoming state: Conduction band in GaAs near Γ along (100).

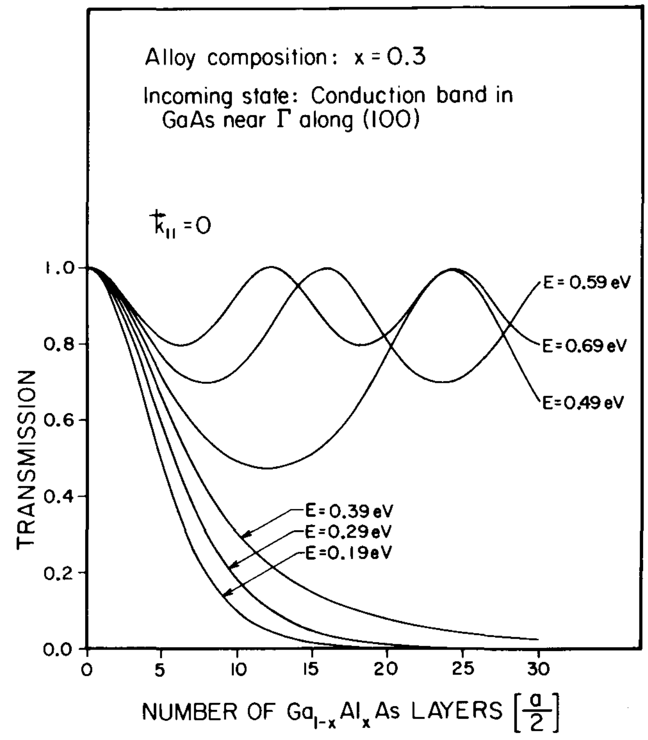

FIG. 3. Total transmission coefficient $T(\mathbf{k}_\parallel, E)$ as a function of central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier thickness for different incoming energies. The incoming Bloch state has no momentum parallel to the interface $\mathbf{k}_\parallel = 0$. The $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ alloy composition is $x = 0.3$. Incoming state: Conduction band in GaAs near Γ along (100).

$E_{\Gamma}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} \approx 0.41$ eV. Transmission through the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier is either tunneling or propagating, depending on the nature of the Bloch states available for strong coupling in the alloy. For energies of the incoming state less than $E_{\Gamma}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, the available states in the alloy are *gap states* (k_{Γ}^{II} complex) and the wave function is damped in the barrier. However, for energies of the incoming state greater than $E_{\Gamma}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, the available states in the alloy are *band states* (k_{Γ}^{II} real) and the wave function is not damped in the barrier.

Generally, when an incoming state in GaAs is derived from a conduction band extremum, say λ, such that $k_0 \equiv k_{\lambda}^{I}$ and $\psi(\mathbf{k}_{\parallel}, k_0) \equiv \psi(\mathbf{k}_{\parallel}, k_{\lambda}^{I})$ the mode of transport (i.e., tunneling or propagating) appears to be determined by the nature of the states in $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ derived from the same conduction band extremum $\psi(\mathbf{k}_{\parallel}, k_{\lambda}^{II})$. For energies of the incoming state less than the alloy conduction band edge $E_{\lambda}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, the states that couple strongly in the alloy are gap states [$\psi(\mathbf{k}_{\parallel}, k_{\lambda}^{II})$ evanescent] and hence the wave function is damped in the barrier. However, for energies of the incoming state greater than the alloy conduction band edge $E_{\lambda}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, the states that couple strongly in the alloy are band states [$\psi(\mathbf{k}_{\parallel}, k_{\lambda}^{II})$ propagating] and hence the wave function is not damped in the barrier.

In the tunneling regime of transport, transmission occurs mostly via the coupling to the alloy Γ-point *evanescent* states (k_{Γ}^{II} complex). As seen in Fig. 3, the evanescent character of the wave function in $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is reflected in the fact that the transmission coefficient $T(\mathbf{k}_{\parallel}, E)$ is an exponentially decaying function of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier thickness. These observations are similar to those obtained from the thick-barrier WKB approximation.[15,16] For incoming states with energy greater than $E_{\Gamma}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, transmission occurs mostly via the coupling to the alloy Γ-point *propagating* states (k_{Γ}^{II} real). The transmission coefficient is unity when the thickness of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier contains an integral number of half-wavelengths (determined by k_{Γ}^{II}) in the barrier region. Under these resonant scattering conditions, the states derived from the conduction band Γ point couple strongly to each other and channeling into Bloch states derived from different conduction band extrema is found to be small. This observation is supported by the original work[1,2] on the transport of Bloch states at a single GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ heterojunction. For energy of the incoming state above $E_{\Gamma}^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, the transmission coefficient is a periodic function of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier thickness. Since the wave vector k_{Γ}^{II} increases with incident Bloch state energy, the period of the transmission amplitude decreases with the energy of the incident Bloch state. The off-resonance transmission amplitudes increase with increasing incident energy. The general qualitative behavior of the transport is similar to that exhibited by plane wave states incident on a rectangular quantum-mechanical barrier.[17]

Figure 4 shows the total transmission and reflection coefficients $T(\mathbf{k}_{\parallel}, E)$ and $R(\mathbf{k}_{\parallel}, E)$ as a function of the number of monolayers forming a central AlAs barrier. The energy of the incoming Bloch state $\psi(\mathbf{k}_{\parallel}, k_{\Gamma}^{I})$ is $E = 0.51$ eV, measured with respect to the GaAs conduction band minimum. The incoming state derived from near the conduction band Γ point has vanishing parallel momentum $\mathbf{k}_{\parallel} = 0$. At this energy the states available for transport in AlAs are *propagating* states near the X-point extremum (k_{X}^{II} real), and *evanescent* states connecting to the Γ point (k_{Γ}^{II} complex) at higher energy. Here again it is found that, for incoming states derived from the GaAs conduction band Γ point, transmission through the AlAs barrier occurs mostly via the coupling to evanescent states that connect to the AlAs conduction band at the Γ point. At small AlAs barrier thicknesses, transmission of conduction band Γ-point incoming states is governed by *tunneling*. In this regime, the incoming state $\psi(\mathbf{k}_{\parallel}, k_{\Gamma}^{I})$ tunnels through the AlAs barrier by coupling to the evanescent Bloch states $\psi(\mathbf{k}_{\parallel}, k_{\Gamma}^{II})$ associated with the conduction band Γ-point minimum. However, it was found that under energetically favorable conditions, transport could exhibit very sharp *resonance scattering* through available propagating X-point states $\psi(\mathbf{k}_{\parallel}, k_{X}^{II})$. This mode of resonant transport occurs for thick AlAs barriers when the tunneling through Γ-point-derived evanescent Bloch states is negligible. Resonance scattering through propagating X-point Bloch states appears to be very sharp due to the weak coupling between $\psi(\mathbf{k}_{\parallel}, k_{\Gamma}^{I})$ and $\psi(\mathbf{k}_{\parallel}, k_{X}^{II})$. Similar regimes of transport have also been reported in the case of GaAs–$\mathrm{GaAs}_{1-x}\mathrm{P}_x$–GaAs strained (100) double heterostructures.[4]

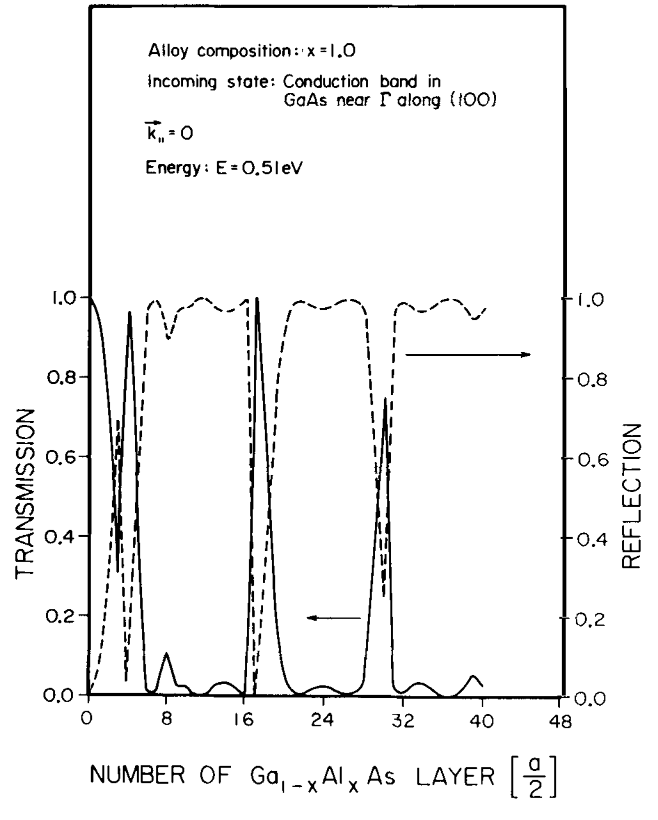

FIG. 4. Total transmission (solid line) and reflection (dashed line) coefficients $T(\mathbf{k}_{\parallel}, E)$ and $R(\mathbf{k}_{\parallel}, E)$ as a function of central AlAs barrier thickness for an energy of $E = 0.51$ eV. Energy is measured with respect to the GaAs conduction band minimum and $\mathbf{k}_{\parallel} = 0$. Alloy composition: $x = 1.0$. Incoming state: Conduction band in GaAs near Γ along (100).

B. Admixture of states of different symmetries

We now analyze the relative contributions of the X-point and the Γ-point conduction band Bloch states to the transmitted wave function as a function of the alloy composition x. Figure 5 shows the transmission coefficients $T_\Gamma(\mathbf{k}_\parallel, E)$ and $T_X(\mathbf{k}_\parallel, E)$ as a function of alloy composition, for two different $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier thicknesses. The energy of the incoming state is $E = 0.69$ eV measured with respect to the GaAs conduction band minimum. For the range of alloy compositions studied, this energy is greater than $E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$. At this energy the Γ-point and X-point states in GaAs and $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ are *propagating* ($k_\Gamma^I, k_\Gamma^{II}, k_\Gamma^{III}$ real, and $k_X^I, k_X^{II}, k_X^{III}$ real). The incoming Bloch state has $\mathbf{k}_\parallel = 0$.

As mentioned above, the Γ-point energy edge $E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}}$, scales linearly with the alloy composition. The composition x is therefore proportional to the Γ-point barrier height at the interface. For the range of alloy compositions studied, the Γ-point energy edge of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ varies approximately in the range $0\ \mathrm{eV} \leqslant E_\Gamma^{\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}} \leqslant 0.47$ eV, above the GaAs Γ-point conduction band minimum. For an energy of the incoming state of $E = 0.69$ eV, the transport regime for incoming states derived from the conduction band Γ point is propagating since the coupling states in the alloy are propagating Bloch states. Since the energy of the incoming state lies above the Γ-point energy edge of the alloy, the transmission amplitude is a weakly dependent function of the barrier height.

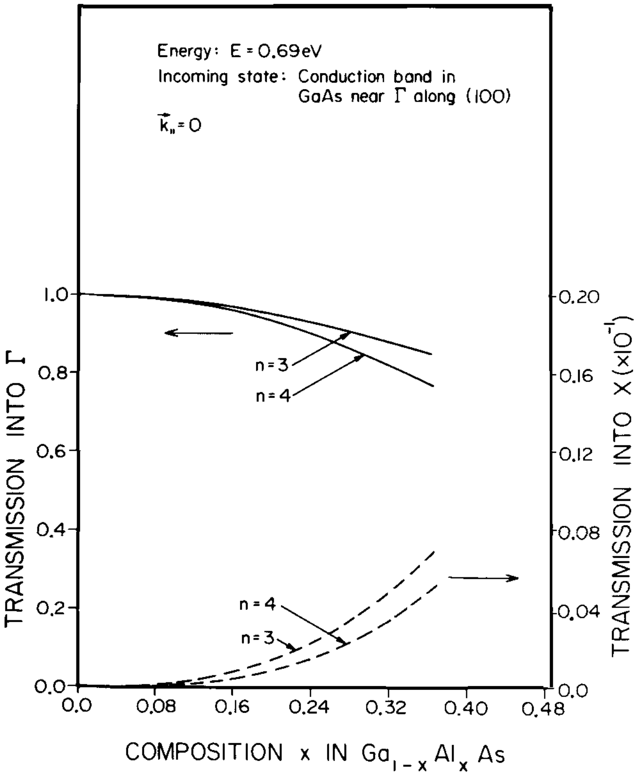

FIG. 5. Wave vector-resolved transmission coefficients $T_\Gamma(\mathbf{k}_\parallel, E)$ (solid line) and $T_X(\mathbf{k}_\parallel, E)$ (dashed line) as a function of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ alloy composition x for different barrier thicknesses. The energy of the incoming state is $E = 0.69$ eV. The number of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier layers is n, and $\mathbf{k}_\parallel = 0$. Incoming state: Conduction band in GaAs near Γ along (100).

As the Al content of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ increases, transmission into the propagating X-point Bloch states $\psi(\mathbf{k}_\parallel, k_X^{III})$ increases but remains rather small. States derived from the same extremum of the conduction band appear to couple strongly to each other across the GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ interface. However, states derived from different extrema of the conduction band appear to couple weakly across the GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ interface.

IV. SUMMARY AND CONCLUSION

We have calculated the transport coefficients of Bloch states through GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$–GaAs double heterojunctions. The model uses complex-k-band structures and transfer matrix methods in the tight-binding approximation. With these techniques, k_z-resolved transport coefficients can be calculated. This, in turn, allows for a better understanding of the transmission coefficients of Bloch states derived from different extrema of the conduction band in GaAs. The incoming electron is derived from the GaAs conduction band Γ point. Calculation of transport coefficients associated with various conduction band valleys were carried through as a function of (1) energy of the incoming Bloch state, (2) thickness of the central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier and, (3) alloy composition x in the central $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier.

States derived from the same extremum of the conduction band appear to couple strongly to each other across the GaAs–$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ interface. Transmission through the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier is either tunneling or propagating depending on the nature of the Bloch states available for strong coupling in the alloy. For energies of the incoming states near the GaAs conduction band Γ point, transmission through the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ barrier occurs mostly via the coupling to states (evanescent or propagating) that connect to the alloy conduction band at the Γ point.

In the propagating mode of transport, resonances in the transmission could possibly be used in GaAs high-speed low-power electronic devices. In an operational mode, it is desirable to populate the low-mass high-velocity GaAs conduction band Γ-point minimum and to depopulate the high-mass low-velocity X and L valleys. These results could provide the basis for an interesting filter for use in high-speed devices.[18]

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