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**"Investigation of Two-Terminal Resonant
Tunneling Devices"**

by

**Colombo R. Bolognesi, B.Eng. (Electrical)
McGill University, Montreal.**

**A thesis submitted to the Faculty
of Graduate Studies and
Research in partial fulfillment
of the requirements for the degree of**

Master of Engineering

**Ottawa-Carleton Institute for Electrical Engineering
Department of Electronics
Faculty of Engineering
Carleton University**

July 1989

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Tunneling Devices"**

submitted by Colombo R. Bolognesi in partial fulfillment of the requirements
for the degree of Master of Engineering.

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ABSTRACT

In tandem with the development of epitaxial growth technologies such as Molecular Beam Epitaxy (MBE) and Metal-Organic Chemical Vapour Deposition (MOCVD) the field of transport through synthetically modulated bandgap structures has generated much interest over the past two decades. These structures can be designed to exploit the wave nature of charge carriers thus opening new horizons for device design. This work represents a theoretical and experimental investigation of two-terminal resonant tunneling devices. A simple model (applicable to multiple well structures) for two-terminal resonant tunneling devices is first developed by solving Schroedinger's equation using Airy functions in conjunction with transfer matrix formalism. The validity of the present approach is demonstrated through the design of test structures which were grown by MBE. Single and asymmetric triple well structures were successfully fabricated. The asymmetric triple well structure is believed to be the first one of its kind to exhibit negative differential resistance at room temperature with a peak current density of 8600A/cm^2 , higher than published data at 300°K . A novel device relying on resonant tunneling of electrons through the virtual states above a multiple quantum well stack is proposed and an attempt is made to observe this phenomenon experimentally. Comparison of experimental data with model predictions demonstrates the usefulness of the present model.

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DEFINITIONS

$Ai(x), Bi(x)$:	Airy and complementary functions.
$D(E_F, V, T)$:	Electron supply function.
e, q :	Electron charge, 1.602×10^{-19} C.
E_F :	Fermi level.
E_D :	Donor ionization energy.
$E_{\Gamma X L}$:	Energy gap for the Γ, X, L bands.
ΔE_g :	Energy gap difference at heterojunction.
ΔE_{cr} :	Γ conduction band discontinuity at heterojunction.
$F_{1/2}(\eta)$:	Fermi integral of order $1/2$ of η .
Γ, X, L :	High symmetry points in reciprocal space.
h :	Planck's constant, 6.634×10^{-34} J-sec.
$\hbar$:	Reduced value of Planck's constant, $h/2\pi$.
J :	Current density (A/cm^2).
k :	Boltzman's constant, 1.381×10^{-23} J/K.
k :	Electron crystal momentum.
m^* :	Electron effective mass.
m_0 :	Free electron rest mass, 9.106×10^{-31} kg.
N_c :	Effective density of states at the conduction band edge.
N_D :	Donor dopant concentration.
n :	Electron concentration.
$p_{ }$:	Momentum parrallel to heterojunction plane, (p_x, p_y) .
$p_{\perp}$:	Momentum perpendicular to the heterojunction plane, p_z .
T :	Absolute temperature ($^{\circ}K$).
$W(a, b)$:	Wronskian of a and b .
$u(r, t)$:	Bloch function.
δ :	Donor spin level degeneracy.
ϵ_0 :	Permittivity of free space, 8.85×10^{-14} F/cm ² .
ϵ_r :	Relative dielectric constant.
$\psi(z)$:	Envelope function.
$\Psi_0(r)$:	Electronic wavefunction.

Chapter One

INTRODUCTION

The field of perpendicular transport, that is, parallel to the growth direction of hetero-epitaxial layers, through semiconductor superlattices and other simpler synthetically modulated bandgap structures has generated much interest following the seminal work of Esaki and Tsu during the early 1970's. The inherent negative differential resistance in the current-voltage characteristics of such structures entertained prospects for millimeter and sub-millimeter wave oscillation, mixing and amplification. The development of an active unipolar heterojunction device, which does not incorporate depletion regions (and hence both vertically and laterally compact), for use in ultrafast and ultrahigh density integrated circuits has generated much effort in Japanese and U.S. laboratories. The growth of ultrathin semiconductor layers with abrupt interfaces by Molecular Beam Epitaxy (MBE) [50,68] and Metal-Organic Chemical Vapour Deposition (MOCVD) [51,52] has permitted the observation of quantum mechanical effects in man-made structures, thus opening a whole new domain of physical scale; quantum well devices provide solid state physicists a new tool in investigating quantum mechanical phenomena. In this chapter the main historical developments in resonant tunneling devices are discussed and an outline of the state-of-the-art in two terminal devices and its extension to potentially more useful three terminal devices is presented. The scope of the work of the thesis is then indicated.

1.1 Historical Review

During the period of 1969-70, Esaki and Tsu first investigated the electronic properties of infinite one-dimensional periodic structures consisting of alternating ultrathin layers of alternating impurity type or of narrow and wide bandgap semiconductors called superlattices. As depicted in figure 1.1 in such a structure the period of the thin layers is smaller than the carrier mean free path, typically 100 to 1000Å, which depends on the temperature, doping and quality of the semiconductor crystal. Esaki and Tsu

realized that the properties of the host crystal would drastically be altered by the presence of quasi two-dimensional quantum states arising from the superlattice potential profile. Indeed, the introduction of the periodic variations of energy gap along the growth axis confines the charge carriers motion in that direction to some degree. The charge carriers then could freely move in the remaining plane in the form of a two-dimensional charge carrier gas. Esaki and Tsu [1] considered doping and compositional superlattices (see figure 1.2), achieved by periodically varying the impurity type or alloy composition of the epitaxial layers, respectively. The resulting superlattice potential disturbs the band structure of the host bulk crystal. Treating the superlattice as a perturbed bulk crystal led Esaki and Tsu to conclude that since the superlattice period "l" in figure 1.2 is much larger than the host crystal lattice constant a_0 , the host crystal Brillouin zone is folded into several minizones with a wavevector size of $2\pi/l \ll 2\pi/a_0$; as shown in figure 1.3, the minizones correspond to a set of allowed conduction subbands -or minibands- separated by mini forbidden gaps. This situation is similar to the one encountered in the Kronig-Penney model for conduction bands in solids, if the superlattice period is smaller than the carrier mean free path. The minibands arising in this fashion are then said to be of quasi two-dimensional nature since the carrier motion becomes partially confined to the directions parallel to the epitaxial growth layer plane.

The narrow wavevector zones of width $2\pi/l$ and the correspondingly narrow energy minibands make it possible for charge carriers to be excited past the E versus k inflexion point of the minizone in figure 1.3 (i.e. into the region of negative effective mass) on application of low electric fields such that an electron can be decelerated by the application of an increasing electric field. Such an effect leads to a region of negative differential resistance in the I-V characteristic of the superlattice that is, past a given voltage, the current through the device will decrease for an increasing applied voltage. Figure 1.4 depicts such an I-V characteristic. The superlattice negative differential resistance has potential for high frequency, (approximately 250 GHz) oscillator applications [1].

Figure 1.1 Quantum regime threshold. Quantum size effects dominate if the superlattice period is smaller than the electron mean free path [50].

Figure 1.2 Doping (a) and compositional (b) superlattice energy band diagrams [50].

Figure 1.3 Energy minibands arise because of the superlattice periodic potential [50].

Figure 1.4 Negative differential resistance region in the I-V characteristic of a superlattice [50].

Since the work of this thesis is concerned with the electronic transport properties of multiple barrier structures (due to energy gap discontinuities associated with alternate layers of differing alloy composition), a brief discussion of how the energy gap of a semiconductor alloy varies as a function of the alloy composition is necessary. In this regard we will focus on the most technologically mature III-V material system GaAs and consider its $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloy where x is the Al mole fraction of the solid solution. GaAs, like most III-V compounds, crystallizes with the zinc-blende crystal structure which can be thought of as two interpenetrating face-centered cubic sublattices offset by one quarter of the unit cell body diagonal. The Ga ion occupies the first sublattice site while the As ion occupies the second sublattice site. This crystal structure defines a Brillouin zone of the crystal in the wavevector space. As seen in figure 1.6 the Brillouin zone is characterized by high symmetry points known as the Γ , L and X points corresponding to specific crystal momenta. For instance, GaAs is known as a direct bandgap semiconductor because its conduction band minimum occurs at the point of zero (0,0,0) crystal momentum, the so-called Γ point. Other local minima in the conduction band occur at the other high symmetry points in the k space (see figure 1.7). The substitution of Al in some Ga sites modifies the crystal lattice periodicity and hence modifies the alloy energy band diagram. Experimentally, the energy gap dependence on the aluminum mole fraction x at the Γ , L and X points are found to be [44] (see figure 1.5)

$$E_{g\Gamma}(x) = 1.424 + 1.247x \quad (x < 0.45) \quad (1.1a)$$

$$E_{g\Gamma}(x) = 1.424 + 1.247x + 1.147(x-0.45)^2 \quad (x > 0.45) \quad (1.1b)$$

$$E_{gX}(x) = 1.900 + 0.125x + 0.143x^2 \quad (1.2)$$

$$E_{gL}(x) = 1.708 + 0.642x \quad (1.3)$$

In 1973, Esaki and Tsu generalized their results to include compositional superlattices of finite extent [2] and Chang et al. demonstrated the negative

differential resistance effect in the I-V characteristic of a 100 period superlattice where each period consisted of a 60Å GaAs well and a 10Å Al_{0.35}Ga_{0.65}As barrier [3]. The experimental observation of resonant tunneling in a double barrier single quantum well had to await further improvements in hetero-epitaxial growth techniques. In 1974, Chang, Esaki and Tsu [4] first reported peaks in the I-V characteristic at 77°K for an AlGaAs/GaAs double barrier diode, associated with resonant tunneling of electrons through the quasi-stationary states of the quantum well. In 1983, Sollner et al. [5] reported a peak-to-valley ratio of 6:1 in the I-V characteristic of a double barrier resonant tunneling diode at 25°K. They used the diode in high frequency detection (2.5 THz) and mixing experiments that suggested that charge transport through the quantum well might be faster than 10⁻¹³ sec. A year later, with further improvements in epitaxial layer quality, Shewchuk et al. [6] reported the first room temperature observation of negative differential resistance in a resonant tunneling diode with a peak-to-valley ratio of 1.3:1 at 300°K and 4:1 at 77°K. That same year, Sollner et al. [7] reported the 18 GHz operation of a quantum well oscillator with a 5μW power output at temperatures as high as 200°K. The following section describes the most important developments since 1984.

Figure 1.5 $\text{Al}_x\text{Ga}_{1-x}\text{As}$ band gap dependence on x [44].

Figure 1.6 High symmetry points in the first Brillouin zone corresponding to the zinc-blende structure [67].

Figure 1.7 GaAs energy band diagram [67].

1.2 State-of-the-art Resonant Tunneling Devices

The present resonant tunneling structures benefit from the maturity of sophisticated epitaxial growth techniques such as Molecular Beam Epitaxy (MBE) and Metal-Organic Chemical Vapour Deposition (MOCVD). Since resonant tunneling is a quantum interference effect, abrupt and defect free hetero-interfaces are required at the junction between the quantum well and the potential barrier material. The typical structure of a double barrier resonant tunneling diode is shown in figure 1.8. A narrow bandgap semiconductor layer forming the quantum well is sandwiched between two wider bandgap semiconductor layers which form the barriers. Generally, the barrier and quantum well material is kept undoped in order to minimize Coulombic scattering which could destroy the phase coherence of resonantly tunneling electrons. The narrow-bandgap-material outside the barriers is kept undoped over a short distance to minimize dopant migration from the heavily doped electrodes into the well and barrier regions.

1.2.1 Two Terminal Devices

1.2.1.1 DC Characteristics

The two most important static figures of merit of a negative differential resistance device are its peak current density J_p and the magnitude of its negative differential resistance $R=-dV/dI$. A high peak current density is necessary to rapidly charge capacitive parasitics for fast device operation whilst a strong negative resistance region is desirable for logic and amplifier/oscillator applications. Also, the maximum available power generated by a negative differential resistance device, an important figure of merit in microwave applications, is given by [7]

$$P_{\max} = \frac{3}{16} \Delta V \Delta I \quad (1.4)$$

Figure 1.8 Typical resonant tunneling structure.

where ΔV (ΔI) is the voltage (current) extent of the negative resistance region of the I-V characteristic.

Table 1.1 shows the highest peak-to-valley current ratios obtained in $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ resonant tunneling diodes at 77°K and 300°K for a given aluminum mole fraction x . Also shown are the corresponding peak current densities and conduction band discontinuities. It can be seen that there is a trend in increasing peak-to-valley ratio with increasing barrier height ΔE_c in the aluminium mole fraction range $x < 0.45$ for which the barrier energy gap remains with Γ symmetry. The conduction band discontinuity ΔE_c for the $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ heterojunctions listed in table 1.1 was assumed to be equal to 60% of the Γ energy gap [53] as given by equation (1.1).

The transport mechanism across mixed band heterojunctions, that is when the well and barrier material bandgap minima have different symmetries in wavevector space, is not well understood at the present time. Although it is well known that the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ energy gap becomes indirect with X symmetry for $x > 0.45$, as shown in figure 1.5, it is not known whether the Γ or X barrier bands confine the quasibound states in mixed band heterojunction quantum wells. However, Bonnefoi et al. [8] and Calleja et al. [9] claim to have observed resonant tunneling through X-confined states. The controversy surrounding mixed band tunneling is beyond the scope of this thesis.

Resonant tunneling has also been observed in a number of material systems other than the $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ system. Table 1.2 is representative of some of the best results obtained in these alternative material systems. Because the $\text{In}_y\text{Ga}_{1-y}\text{As}$ energy bandgap remains direct (Γ -symmetry), for $0 < y < 1$, but reduces with increasing indium content, a deeper quantum well is obtained if the GaAs well is replaced with an $\text{In}_y\text{Ga}_{1-y}\text{As}$ well. Moreover, InGaAs is lattice mismatched when grown on a GaAs substrate; such a system has strains associated with it and is called pseudomorphic if no misfit dislocations are present in the strained layers. A good introduction to the effects of lattice mismatch on epitaxial growth can be found in reference [58].

Briefly, if the misfit between a growing layer and the substrate is sufficiently small, the first atomic layers to be deposited will be strained to match the substrate and the strain will be accommodated coherently that is, without dislocations. As the epitaxial layer grows its rigidity increases and past a critical thickness h_c the strain energy is so large that it becomes energetically favorable for misfit dislocations to be introduced in order to accommodate the strain. Appendix A illustrates the variation of energy gap and lattice constant with composition for III-V semiconductors. A controllable well depth can be used to tune the voltage V_p of the peak current without widening the quantum well, allowing more electrons to maintain the phase coherence required for resonant tunneling since an electron traversing a thinner well is less likely to suffer scattering than when traversing a wider well [10]. The deepening of the quantum well is also believed to improve the peak-to-valley ratio by increasing the Γ -X valley separation between the well and barrier thus suppressing the valley current component transported via the X-band [11,17]. GaAs is not the only possible choice for substrate material. Indeed, because $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and $\text{Al}_{0.48}\text{In}_{0.52}\text{As}$ are lattice matched to InP, they may be grown free of strain induced dislocations on InP substrates. The small effective mass in AlInAs barriers is believed to enhance the barrier transmission coefficient while the low Schottky barrier height associated with contacts to InGaAs leads to low resistivity non-alloyed ohmic contacts [48,49]. In this material system, band mixing problems at the barrier/well heterojunctions are avoided since the AlInAs barriers have a direct energy gap for aluminium concentration of up to 70% [44]. Broekaert et al. [12] took this type of structure a step further by replacing the lattice matched $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ quantum well with a deeper, pseudomorphic, InAs well. They reported a record current peak-to-valley ratio of 30 (63) at 300°K (77°K) with a peak current density of 6000 A/cm² both at 77°K and 300°K. AlSb/InAs heterojunctions provide a large (1.8 eV) Γ barrier to conduction band electrons and have therefore recently been used to implement AlSb/InAs/AlSb resonant tunneling diodes [13]. The low effective mass in InAs permits the use of wider wells while still maintaining well defined quasibound states in the well, thus making the contacting of the well region more feasible [13] for potential

Aluminum mole fraction x .	ΔE_c (eV)	P/V 300/77K	J_p (A/cm ²) 300/77K	Ref.
0.25	0.18	1.3/4.0	1700/2200	[6]
0.40	0.28	-/13.1	-/11.0	[59]
0.42	0.31	3.9/14.3	6346/8654	[60]
1.0	0.98	3.5/10.0	40000	[61]

Table 1.1 Some of the best results obtained with $Al_xGa_{1-x}As$ resonant tunneling diodes.

Barrier/Well Material.	ΔE_c (eV)	P/V 300/77K	J_p (A/cm ²) 300/77K	Ref.
$Al_{0.35}Ga_{0.65}As/In_{0.20}Ga_{0.80}As$	0.595	-/6.0	-/-	[62]
$AlAs/In_{0.10}Ga_{0.90}As$	1.70	1.5/13.0	510	[10]
$AlAs/In_{0.53}Ga_{0.47}As$ *	2.158	14.0/35.0	23000	[63]
$Al_{0.48}In_{0.52}As/In_{0.53}Ga_{0.47}As$ *	0.627	-/11.4	-/55000	[64]
$Al_{0.48}In_{0.52}As/In_{0.53}Ga_{0.47}As/InAs$ *		30.0/63.0	6000	[12]
$AlSb/InAs$	1.80	1.8/9.0	355	[13]

Table 1.2 Alternative material systems for resonant tunneling diodes (*: grown on InP substrate).

resonant tunneling transistor applications (in comparison, GaAs wells are too thin to be contacted).

These results can be compared to the ones obtained for the conventional pn junction tunnel diode also known as the Esaki diode. The best room temperature peak-to-valley ratios for $\text{Al}_x\text{Ga}_{1-x}\text{As}$ resonant tunneling diodes are comparable to the ones obtained with silicon and indium arsenide Esaki diodes which typically exhibit a peak-to-valley ratio of 4:1 and 2:1 respectively at 300°K [27]. The peak-to-valley ratio figures for alternate material systems vary a lot but the results achieved by Broekaert et al. [12] compare favorably with the values obtained for germanium (8:1), gallium arsenide (12:1) and gallium antimonide (12:1) Esaki diodes [27].

1.2.1.2 High Frequency Characteristics

Frensley [14,15] performed quantum transport calculations which show that the resonant tunneling process (transport through the quantum well) takes place in times of the order of 10^{-13} sec. In particular, his calculations show that the intrinsic (that is without parasitics) negative conductance and nonlinear response of a resonant tunneling diode can persist up to 6THz and 10THz respectively (1THz = 1000GHz). These calculations lend support to Sollner's report of signal detection at frequencies as high as 2.5THz [5]. Frensley [14] showed that, without capacitive parasitics, current switching from the peak to the valley of the I-V characteristic could typically be achieved in times of the order of 250fs (0.25×10^{-12} sec); more recent work by Diamond et al. [16] pointed out that in reality the switching time of a resonant tunneling diode is limited by the device RC time constant associated with the device contact resistance and depletion region capacitance as opposed to the quantum well dwell time (the time for which the probability density of a tunneling electron is peaked in the quantum well) and to the depletion layer transit time. According to Diamond, properly designed devices should be characterized by switching transition times below 5ps.

Brown et al. [17] reported fundamental oscillations up to 201GHz at room temperature using a 4 μ m diameter AlAs/GaAs/AlAs resonant tunneling diode mesa mounted in a rectangular waveguide resonator. The diode consisted of 17Å AlAs barriers sandwiching a 45Å well with moderately doped electrodes, and had a room temperature current peak-to-valley ratio of 3.5:1. The same group also proposed an improved device, with an optimized electrode doping profile, with expected oscillation around 640GHz for a 1 μ m mesa geometry [17].

1.2.1.3 Device Applications

Aside from the negative resistance amplifier/oscillator and multilevel logic applications, two terminal resonant tunneling devices have shown potential for application in both analog and digital signal processing. For example, Lakhani et al. [18] have demonstrated a 11-bit parity generator using a single active device (and one resistor). The active device, in the form of five vertically integrated AlInAs/InGaAs resonant tunneling diodes (VIDs) performs the same function as a conventional circuit implementation involving 10 exclusive OR gates. This illustrates that the sequential switching of "m" stacked resonant tunneling diodes can provide bit parity for a 2m+1 bit word. Sen et al. [19] have demonstrated that the parallel combination of 2 resonant tunneling diode can be used for 4-bit word parity generation, frequency multiplication, as a 3-state memory cell and for waveform scrambling purposes at 100°K. In all cases the use of resonant tunneling devices led to a reduced circuit complexity in comparison to the conventional switching transistor circuit implementation of the same function. These examples demonstrate that resonant tunneling diodes have potential for application in many fields. However, their technology is still at an exploratory stage because, in some cases, room temperature operation has yet to be achieved and because reliability considerations have not yet been addressed.

1.2.2 Three Terminal Resonant Tunneling Devices

The extension of resonant tunneling principles to 3 terminal devices, while providing some input to output isolation, results in transistors capable of performing higher order primitive functions rather than the simple logic level switching of conventional transistors. Therefore, the study of resonant tunneling transistors is of interest for high density, high speed integrated circuit applications.

1.2.2.1 Resonant Hot Electron Transistor (RHET)

In 1985, Yokoyama et al. [20] proposed and demonstrated a unipolar GaAs/AlGaAs Resonant Hot Electron Transistor (RHET) in which electrons are injected from the emitter into the base by resonant tunneling through a quantum well structure located at the emitter/base junction. The injected electrons enter the collector near ballistically over a bias dependent barrier at the base/collector junction. Figure 1.9 shows the RHET operation principle: for a suitable emitter-base bias the collector current exhibits a peak with respect to V_{EB} due to the resonant tunneling of electrons from the emitter into the base. Any increase (or reduction) in V_{EB} results in a collector current drop as the quantum well is taken out of the resonance condition; the device therefore exhibits a negative transconductance when the emitter-base bias is increased beyond the peak current bias point. The GaAs/AlGaAs RHET suffers from a low common emitter gain of 5 [21] due to hot electrons thermalizing with various scattering processes in the base and not having enough energy to overcome the collector barrier. The same workers reported a InGaAs/In(AlGa)As RHET lattice matched to a semi-insulating InP substrate operating at 77°K, with a collector peak current density $J_p = 2.8 \times 10^4$ A/cm² and a peak-to-valley current ratio of 15 [22]. It is believed that the increased Γ -L valley separation in InAs (0.78eV compared to 0.30eV in GaAs) and a graded collector barrier (to reduce quantum mechanical reflection at the collector) helped to increase the common emitter gain to 25.0 for a 250Å thick base. Figure 1.10 illustrates the

Figure 1.9 RHET operation principle [20].

Figure 1.10 Collector current characteristics for a 250Å base RHET [22].

collector current characteristics for this device. The emitter-to-collector time delay τ_{EC} for the RHET was estimated to be 2.4ps [22] corresponding to a f_T of 66GHz, illustrating the RHET potential for high speed applications. Frequency doubler [20], exclusive NOR gate [20] and flip-flop [23] circuits have been demonstrated: all used a single RHET along with a few resistors to implement these higher order primitive functions with a much reduced circuit complexity when compared to their conventional circuit implementations. An improvement in the RHET common emitter current gain can be achieved by replacing the collector barrier with a reverse biased pn junction thereby ensuring that both hot and thermalized electrons reach the collector. The common emitter current gain (20 at 77°K) improvement is believed to be owed to the absence of a collector barrier to oppose the efficient collection of low energy electrons.

1.2.2.2 Resonant Tunneling Bipolar Transistor (RTB)

Since the application of an electric field directly across a double barrier structure reduces its peak transmission coefficient to a value smaller than 1.0 by destroying the quantum well symmetry, an improved peak-to-valley current ratio should be obtained for a device in which the quantum well region is kept under flat band conditions. Capasso et al. [24] proposed a Resonant Tunneling Bipolar transistor (RTB) that essentially consists of a Heterojunction Bipolar Transistor (HBT) with a quantum well resonator inserted in the base region (see figure 1.11). In the RTB, the negative transconductance is achieved by minority carrier injection into the quantum well quasi-stationary states rather than by the application of an electric field directly across the quantum well resonator. Capasso et al. [25] were the first to demonstrate the resonant tunneling transistor action at room temperature with a common emitter gain of 7. In the common emitter configuration, the RTB acted as an oscillator when biased in its negative conductance region. The fundamental frequency was 20MHz but higher oscillations frequencies are expected (>10GHz) for optimized collector bias circuits and probe stages.

	EMITTER	BASE	COLLECTOR
X	.25	.24 .07 .01 .0	0
dopant	n	n p p n n n p	n

Figure 1.11 Resonant Tunneling Bipolar Transistor [25]

1.3 Thesis Work

This work is a theoretical and experimental investigation of two terminal resonant tunneling devices. The analysis of transport through resonant tunneling structures is treated by solving a single electron Schroedinger equation using an envelope function approximation. Rather than undertaking a numerically intensive fully self-consistent solution of both Schroedinger's and Poisson's equations, a uniform electric field is assumed to entirely support the voltage applied to the device. This simplified approach to the modeling of resonant tunneling structures is put to use in the design of a simple double barrier single quantum well resonant tunneling diode and of novel asymmetric multiple quantum well tunneling structures necessitating the alignment of misaligned quasibound states associated with neighbouring quantum wells. These structures were grown by Molecular Beam Epitaxy (MBE) and processed into two terminal devices. It was found that the model can satisfactorily account for the most important features that appear in the experimental results. Furthermore, the fact that some non-trivial structures have been successfully designed and fabricated using the present model suffices to establish it as an excellent first order analysis tool for resonant tunneling device exploration and design.

Among other results we present, to the best of our knowledge, the first room temperature demonstration of the negative differential resistance associated with resonant tunneling through three quantum wells, and this with a record high current density for a resonant tunneling structure of this thickness. We also introduce a new concept in attempting to achieve resonant tunneling through the virtual states of a short-period variably-spaced multiple quantum well stack confined by higher AlAs barriers.

The thesis content is organized in the following manner. Chapter 2 first lays out the basic principles of resonant tunneling. Chapter 3 establishes the model used in this work. The application of the envelope function approximation in heterostructures is considered first. Its use in the calculation of the transmission coefficient through multibarrier structures

using the Airy function and transfer matrix formalism is then worked out for constant electric fields across the barrier and quantum well regions. Chapter 3 ends with a brief discussion of the current density calculation and of the numerical implementation of the model. Chapter 4 is used to illustrate the application of the present modeling approach via examples. To date, there has been little information regarding the use of Airy functions in the modeling of resonant tunneling devices with the exception of Brennan's work [34]. However, Brennan's results showed significant discrepancies with the previously numerically computed results of Vassel et al. [35], thereby undermining the credibility of Airy function solutions. In Chapter 4, the source of these discrepancies is pointed out for the first time and the two approaches are reconciled. Chapter 5 presents the design of the devices to be investigated experimentally, including the novel structure referred to above. Chapter 6 covers the experimental work pertaining to MBE growth and device processing and reports the experimental results obtained. Chapter 7 concludes this work and outlines possibilities for further research.

Chapter Two

RESONANT TUNNELING PRINCIPLES

2.1 Tunneling through a rectangular potential barrier

Much insight into the resonant tunneling phenomenon can be achieved by first considering tunneling through the simplest of potential profiles: a rectangular potential barrier of height eV_0 and thickness a . According to Newtonian mechanics, an incident particle of energy E and mass m is always reflected by the barrier if $E < eV_0$. Indeed, in the realm of classical mechanics, a negative kinetic energy and an imaginary momentum preclude any penetration of the barrier region by the particle. Still, if $E > eV_0$, classical mechanics predict that the particle is always transmitted over the barrier albeit with a change in velocity. A plot of the transmission coefficient then yields a step function with a discontinuity at $E = eV_0$. On the other hand, the application of wave-mechanical methods to the same problem allows exponentially damped wavefunctions to penetrate and eventually traverse sufficiently thin classically forbidden regions, giving rise to the well-known "tunnel effect" - a direct consequence of the wave nature of matter.

The ratio of the transmitted (reflected) to the incident probability current density is known as the barrier transmission (reflection) coefficient T (R). The conservation of probability current density requires that $R + T = 1$. Analytical solutions are generally possible for very simple potential profiles such as the rectangular potential barrier of figure 2.1. Most quantum mechanics textbooks (see reference [45] for example) show that the transmission coefficient of a particle (from here on electron will be used in the place of particle) through the barrier, shown in figure 2.1, is given by

$$T = \frac{\hbar k_3 / m}{\hbar k_1 / m} = \left(1 + \frac{\sinh^2(k_2 a)}{4 \frac{E}{V_0} \left[1 - \frac{E}{V_0} \right]} \right)^{-1} \quad (2.1)$$

Figure 2.1 Rectangular barrier potential profile.

Figure 2.2 Transmission coefficient through a $30\text{\AA}$ 0.3eV barrier for effective masses equal to $0.0067m_0$ (solid), $0.067m_0$ (dotted) and $0.670m_0$ (dashed) as a function of energy.

where

$$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (2.2)$$

for $E < V_0$. A plot of the transmission coefficient through a 1eV barrier for an electron incident on the barrier with an energy of 0.3eV is displayed in figure 2.2, with the electron mass m as a parameter. The barrier thickness is taken as 30Å and the electron mass was taken as $m=0.0067m_0$, $0.067m_0$ and $0.670m_0$ where $m_0=9.1 \times 10^{-31}$ kg is the free electron rest mass. Figure 2.2 illustrates that for any given barrier height, thickness and incident particle energy, the barrier transmission coefficient is enhanced by a low particle mass. Similarly, the thinning of the barrier enhances the transmission coefficient as can be verified from equation (2.1).

2.2 Resonant tunneling: The Double Barrier Profile

Consider two closely spaced barriers, such as the ones shown in figure 2.3. Suppose that the width of the region separating the barriers (a quantum well) is of the order of the electronic deBroglie wavelength $\lambda = p/\hbar$ where p is the electron momentum and $\hbar$ is Planck's constant. The quantum size effects in this structure give rise to the quantization (similar to case of the particle in a one-dimensional potential box) of the electron energy in the quantum well into discrete quasibound states corresponding to the quantum well energy eigenvalues. The states are referred to as quasibound (or quasi-stationary) because the finite barrier thickness and height lead to a nonzero barrier transmission coefficient, therefore allowing the wavefunction corresponding to a particle to leak out of the well. The double barrier potential profile is electrically transparent to electrons incident with an energy equal to a quantum well eigenvalue, irrespective of the individual barrier widths. Electrons that satisfy this condition are said to resonantly tunnel through the double barrier profile. Physically, the phenomenon may be understood in terms of a constructive interference pattern between those wavefunctions

leaking out of the well (quasibound state eigenfunction) and those incident on the double barrier system; the net effect is the cancellation of the reflected waves only leaving a transmitted wave. Electrons with an energy greater or lesser than a quantum well eigenvalue are said to be off resonance and experience a strong damping. As one might expect intuitively, the total attenuation of non-resonant wavefunctions through the double barrier is dominated by the product of the attenuations of each barrier taken independently [26].

This peculiar behaviour of the transmission coefficient dependence on the energy of the incident particle may be better understood with the aid of an analogy between the double barrier system and the Fabry-Perot optical resonator, its optical analogue. The Fabry-Perot optical resonator consists of two parallel, partially reflecting mirrors separated by a distance w . The problem of a particle incident on the double barrier, where the barriers are characterized by the transmission and reflection coefficients t_1, r_1 and t_2, r_2 for the first and second barriers respectively, is analogous to having a monochromatic wave of radian frequency ω , incident on the two partially reflecting mirrors making up the Fabry-Perot resonator. In the double barrier system, the total probability density must be conserved so that the incident probability density current must be equal to the sum of the reflected and transmitted probability current densities. Similarly, for the optical Fabry-Perot resonator, the incident power density must be equal to the sum of the transmitted and reflected power densities. For illustrative purposes, the transmission coefficient through the double barrier system can be computed by treating the quantum well as a cavity consisting of two parallel, partially reflecting mirrors separated by a distance w . Each barrier is characterized by a reflection coefficient r_i and a transmission coefficient t_i relating the amplitudes of the reflected and transmitted waves to the amplitude of the wave describing the incident particle. The subscripts denote the barrier encountered. Describing the incident particle by a plane wave and considering the infinite number of partial waves produced by the reflections at both barriers yields,

Figure 2.3 Multiple reflections in the double barrier.

$$t = t_1 t_2 e^{ikw} + t_1 r_2 r_1 t_2 e^{i3kw} + t_1 (r_2 r_1)^2 t_2 e^{i5kw} + \dots \quad (2.3)$$

$$t = t_1 t_2 e^{ikw} \sum_{n=0}^{\infty} (r_1 r_2 e^{i2kw})^n \quad (2.4)$$

$$t = \frac{t_1 t_2 e^{ikw}}{1 - r_1 r_2 e^{i2kw}} \quad (2.5)$$

for the amplitude transmission coefficient. Multiplying t by its complex conjugate t^* yields the probability density transmission coefficient T .

$$T = t t^* = \left\{ \frac{|t_1|^2 |t_2|^2}{(1 - r_1 r_2 e^{i2kw})(1 - r_1^* r_2^* e^{-i2kw})} \right\} \quad (2.6)$$

For simplicity, assume both barriers are identical and that the t_i 's and r_i 's are real. Then,

$$\begin{aligned} \Gamma &= |t_1|^2 = |t_2|^2 \\ \rho &= |r_1|^2 = |r_2|^2 \end{aligned} \quad (2.7)$$

and

$$T = \frac{\Gamma^2}{1 + \rho^2 - 2\rho \cos(2kw)} \quad (2.8)$$

which is equal to unity when the spacing between the barriers is an integer multiple of the incident electron wavelength. Figure 2.4 illustrates the effect

Figure 2.4 Effect of the individual barrier reflection coefficient on the double barrier transmission ($p=0.1$ for solid, 0.5 dashed and 0.9 dotted lines).

Figure 2.5 Transmission coefficient through one (solid) and two (dashed) $30\text{\AA}$ 0.35eV barriers. The electron mass was taken as $0.067m_0$ and the quantum well width was taken as $90\text{\AA}$.

of the individual barrier opacity (reflection coefficient) ρ , on the overall transmission coefficient of the double barrier system as determined by equation (2.8). Higher and thicker barriers contribute to a more efficient suppression of off-resonance transmission coefficient leading to very sharp resonances; this effect should contribute to stronger negative differential resistance in a resonant tunneling device through a more efficient suppression of the non-resonant tunneling current.

2.3 The Origin of Negative Differential Resistance

As seen in the previous section, resonant tunneling through a double barrier structure occurs if the longitudinal energy component of an incident electron wave matches the energy eigenvalue of an unoccupied state with the same lateral momentum in the quantum well. Let us consider, with the aid of figure 2.6, how the negative differential resistance arises the I-V characteristic. At low applied voltages the current is small because most of the incident electron distribution is confined to energies smaller than the negatively biased electrode Fermi level plus $k_B T$. Few electrons reach the first quantum well quasibound state and most incident wavefunctions corresponding to the tunneling electrons experience a strong attenuation, hence a low value of transmission coefficient through the double barrier. An increase in the applied voltage lowers the quasibound states with respect to the cathode Fermi level and drastically increases the number of electrons that can resonantly tunnel, thus increasing the current through the device. The current reaches its peak value at a voltage V_p , which brings about the alignment of the emitter conduction band edge to the first quasibound state. Within the first order analysis, $V_{p1} = 2E_1/q$ for a device with symmetric barriers. Experimentally, the observed peak current voltages are generally larger than $2E_1/q$ due to the presence of a significant amount of band bending associated with a charge accumulation layer at the emitter barrier (i.e. the first barrier a tunneling electron encounters), and a depletion layer in the collector region immediately following the second barrier. A further increase in the applied voltage destroys the resonance condition for most electrons and therefore quenches

Figure 2.6 Resonant tunneling process.

the total current flow in the device leading to a negative differential resistance in the I-V characteristic of the double barrier diode. The same sequence of events subsequently applies for the higher quasibound quantum well states (any quantum well must contain at least one state) so that in principle, a double barrier structure incorporating N quasibound states will produce an I-V characteristic with N negative differential regions. For large applied voltages, the emitter barrier resembles a triangular potential barrier and the current through it increases rapidly due to Fowler-Nordheim-like tunneling [27].

2.4 Coherent *versus* Sequential Resonant Tunneling

Up to this point, our discussion of resonant tunneling through a double barrier has assumed that the phase coherence of the tunneling wavefunction is maintained throughout the tunneling process (i.e. Fabry-Perot like resonant tunneling). However, in semiconductors, both elastic and inelastic scattering can destroy the wavefunction phase coherence; this prevents the wavefunction build-up in the quantum well necessary for Fabry-Perot resonant tunneling. Luryi [28] pointed out that the Fabry-Perot constructive interference mechanism is not necessary in order for negative differential resistance to be observed. Instead, a sequential tunneling, which is tunneling through the first barrier into the reduced dimensionality quantum well region and then out through the second barrier, is sufficient to produce the negative differential region in the I-V characteristic. Let us consider sequential tunneling with the aid of figure 2.7. Let z be the direction of tunneling transport. Assuming that the barriers are planar and free of impurities and inhomogeneities, the lateral electron momentum (p_x, p_y) must be conserved upon tunneling into the quantum well. Figure 2.7 depicts the Fermi sphere representing the incident carriers in the degenerately doped emitter electrode. The energy and lateral momentum conservation rules imply that tunneling through the unoccupied quasibound state E_0 is possible only for the electrons with energy $E_c < E_0 < E_F$ and whose momenta lie in a disk corresponding to $k_z = k_0$ where $E_0 - E_c = \hbar^2 k_0^2 / 2m^*$. Such a tunneling current reaches a peak when the shaded disk reaches the Fermi sphere equatorial

plane. At still higher bias, that is when $k_0^2 < 0$, no electrons can tunnel through into the quantum well from the emitter while still conserving their lateral momentum, causing an abrupt drop in the total tunneling current.

Following the work of Stone and Lee [29], Capasso et al. [30] argued that the overall effect of collisions is to decrease the peak transmission through the double barrier by the ratio $\tau_0/(\tau_0 + \tau)$. Here, τ is the reciprocal of the total scattering rate due to the elastic scattering by carriers, impurities and epitaxial layer inhomogeneities as well as inelastic scattering by phonons and $\tau_0 = \hbar/\Gamma$, where Γ is the full width at half maximum (FWHM) of the resonant level E_0 . Mendez showed [31] that the peak current should be roughly proportional to the peak transmission coefficient; the peak current should therefore be directly affected by the amount of scattering in the quantum well.

In sharp contrast with the previous discussion, Jonson and Grincwajg [32] used a variable coherency model to determine that the double barrier dc I-V characteristic should not depend on which tunneling mechanism dominates as long as the quasibound states are well defined in energy (i.e. sufficiently separated). Similarly, Weil and Vinter [33] showed the equivalence of fully sequential and fully coherent tunneling as far as the dc I-V characteristics for resonant tunneling diodes are concerned. To summarize, although the controversy between sequential and coherent tunneling has not yet been fully resolved it, however, seems clear that Fabry-Perot-like tunneling should prevail if the intrinsic quasibound level width Γ is much greater than the scattering induced broadening $\hbar/\tau$. This situation is expected to occur in thin barrier structures since the higher transmission coefficient through the barriers leads to wider resonant level widths [30].

Figure 2.7 Negative differential resistance through momentum conservation.

Chapter Three

MODELING OF RESONANT TUNNELING STRUCTURES

This chapter is concerned with the choice and implementation of a model to be used to compute the transmission coefficient and current density through resonant tunneling structures using, as a starting point, the envelope function approximation [36,42]. The present model should provide enough information to be useful in the design of non-trivial structures at the cost of a reasonably moderate computational effort.

Let z be the direction of transport. A full solution of Schroedinger's (under the envelope function approximation) and Poisson's equations - hereafter referred to as the self-consistent solution- in multibarrier structures has already been performed [54,55]. Given an applied voltage to the device of interest, the self-consistent solution begins with a guessed potential profile; very often the initial profile is that of a uniform electric field through the entire structure. The transmission coefficient is then computed as a function of energy and the envelope wavefunction $\psi(z)$ is calculated throughout the device structure. The electron charge density is then found as

$$\rho(z) = q \sum_{E_i} |\psi(E_i, z)|^2 f(E, E_F) \quad (3.1)$$

where $f(E, E_F)$ is the Fermi Dirac distribution

$$f(E, E_F) = 1 / (1 + \exp\{([E_i + \hbar^2 k(z)^2 / 2m^* - E_F] / kT)\}) \quad (3.2)$$

The resulting charge density is then substituted in a one-dimensional Poisson equation

$$\frac{d}{dz}(\epsilon(z) \frac{d}{dz} \phi(z)) = \rho(z) \quad (3.3)$$

from which both the potential $\phi(z)$ and electric field $F(z)$ are obtained. Schroedinger's equation is then solved once again using the new potential

profile whence providing an updated version of the transmission coefficient as a function of energy. The program then loops back and recalculates $\psi(z)$, $\rho(z)$, $\phi(z)$ and $F(z)$ until satisfactory convergence is reached. This whole process must be carried out at each bias point during the calculation of an I-V characteristic.

Clearly, the self-consistent method is very computer intensive. Brennan [54] pointed out that the self-consistent potential only influences the transmission coefficient computation for high doping levels ($>10^{18} \text{ cm}^{-3}$) in the well and barrier regions. Band bending in the form of an accumulation region at the cathode barrier (emitting barrier) as well as a depletion region immediately following the anode barrier always act to shift the negative differential conductance region to higher voltages. In other words, the inclusion of self-consistency effects amounts to the application of a smaller voltage directly across the quantum well. Indeed, the use of a uniform electric field across undoped quantum well and barrier regions obscures none of the essential physics of the tunneling transport whilst making the program a good deal less numerically intensive.

The present model involves first calculating the transmission coefficient through the multiple barriers by using an Airy function [40] solution to the effective mass Schroedinger equation in an envelope function approximation [36,42] describing the multibarrier tunneling structure in a uniform electric field. The Airy function is usually known for its application to the problem of radio wave propagation around the earth's surface [43]. The combination of the Airy function and of the transfer matrix formalism developed in section 3.4 has the merit of providing an exact analytical solution for the transmission coefficient T at a given incident energy, and of being mathematically elegant.

3.1 Model Description

Traditionally, the analysis of semiconductor devices has been carried out with the aid of macroscopic parameters such as the carrier mobilities,

diffusion coefficients and lifetimes. These parameters are determined by the macroscopic average of microscopic phenomena in the semiconductor material. As the device dimensions under consideration shrink below $1\mu\text{m}$, the averaging out of the microscopic effects is incomplete and the above macroscopic parameters lose their relevance for the device analysis. The advances in epitaxial growth techniques, such as MBE and MOCVD have made the controlled growth in the z-direction of microscopic structures ($\leq 20\text{\AA}$) possible while the progress in high resolution lithography now permits the definition of submicrometer patterns in the (x,y) plane. Since these dimensions are comparable to the electronic deBroglie wavelength in high quality semiconductor crystals, quantum phenomena are expected to play a major role in the device behaviour of such small structures; hence the transport mechanism should be described by a Schroedinger-like equation.

This work is primarily concerned with the transport properties in the perpendicular direction to the heteroepitaxial layer plane, the z-direction, assuming that the properties of the layers are translationally invariant in the (x,y) plane. Explicitly, we shall model resonant tunneling devices by making the following basic assumptions:

- (i) The electron transport is a one-dimensional process, that is, all parameters are kept constant throughout any epitaxial layer (that is, in directions normal to that of transport). The epitaxial layers are modeled by abruptly varying effective masses and conduction band edges in the longitudinal (z) direction.
- (ii) Transport is unipolar, that is, all the current contributions come from electron transport only.
- (iii) All scattering phenomena and electron-electron interactions are neglected. The electron transport is therefore modeled in a single-electron approximation.
- (iv) Tunneling is specular; that is, in tunneling, electrons conserve both total energy and particle momentum parallel to the epitaxial layer planes

$p_{||}=(p_x, p_y)$. In the case of planar junction geometries most analyses are based on this boundary condition [71].

(v) Propagating and evanescent states are described in a stationary (time independent) single band envelope function approximation (to be discussed in the following section).

(vi) Band non-parabolicity is neglected so that the effective mass in each layer is constant with increasing energy.

(vii) The heavily doped contacts surrounding the barrier and quantum well material remain in local thermodynamic equilibrium when a bias is applied to the device. The Fermi level separation between the electrodes is equal to the applied voltage.

(viii) The barrier and quantum well material is undoped and therefore supports a constant electric field (neglecting the difference in the dielectric constant between the barrier and well material); the effect of the electrons in the quantum well is neglected. This last assumption is justified if the electron density in the well is small compared to the electron concentration in the electrodes.

3.2 The Envelope Function Approximation

The envelope function approximation [36,42] is the most commonly used tool in the description of electronic states in quantum wells and superlattices because of its convenience and computational simplicity. A brief description of its origins and limitations is given prior to considering its application pertaining to this work. We begin by considering the well known treatment of electrons in bulk semiconductor crystals. In the single electron approximation, the energy states of an electron in the crystal are described by a wavefunction $\Psi_0(\mathbf{r},t)$ which is determined by the solution to the Schrodinger equation [36]

$$i\hbar \frac{d\Psi(\mathbf{r},t)}{dt} = H\Psi(\mathbf{r},t) + U(\mathbf{r},t)\Psi(\mathbf{r},t) \quad (3.4)$$

where H is the Hamiltonian operator

$$H = \frac{-\hbar^2 \nabla^2}{2m_0} + U_L(\mathbf{r}) \quad (3.5)$$

and $U_L(\mathbf{r})$ is the periodic potential due to the lattice ions, $U(\mathbf{r},t)$ is the sum of the macroscopic potential U_E (a solution to Poisson's equation) and the scattering potential U_S (which is set to zero according to point (iii) above), $\hbar$ is the reduced value of Planck's constant and m_0 is the free electron mass. The eigenfunctions of the Hamiltonian operator H are given by

$$H\Phi_{v,k}(\mathbf{r}) = E_v\Phi_{v,k}(\mathbf{r}) \quad (3.6)$$

where v is the band index and k is the electron wavevector, a quantity related to the electron crystal momentum p through $p = \hbar k$. The functions $\Phi_{v,k}(\mathbf{r})$

$$\Phi_{v,k} = e^{ikr} u_{v,k}(\mathbf{r}) \frac{1}{\sqrt{\Omega}} \quad (3.7)$$

where Ω is the volume of normalization, are known as the Bloch functions and $u_{v,k}(\mathbf{r})$ has the periodicity of the crystal lattice (just as does $U_L(\mathbf{r})$) and resemble the atomic wavefunctions in the vicinity of the lattice ions. The $E_v(k)$ relationships can be plotted for some specific wavevector orientations to produce the semiconductor energy band diagram as in figure 1.7 for example.

Clearly, attempting to directly solve the original Schroedinger equation across heterojunctions in heterostructures and superlattices with the potential profile changing from one material to the next is a formidable task. Instead, one uses an effective mass Schroedinger equation in the form of the envelope function approximation and seeks solutions to [36]

$$i\hbar \frac{d\Psi(\mathbf{r},t)}{dt} = \frac{-\hbar^2 \nabla^2}{2m^*} \Psi(\mathbf{r},t) + E_d(\mathbf{r},t)\Psi(\mathbf{r},t) + U_s(\mathbf{r},t)\Psi(\mathbf{r},t) \quad (3.8)$$

which are obtained by modeling the different material layers by a varying conduction band edge $E_c(r)$ and effective mass m^* . It can be shown [36] that this approximation is valid if, (1) the macroscopic potential is nearly constant over a unit cell and, (2) $u_{v,k}(r) \approx u_{v,k'}(r)$ that is, if the periodic parts of the Bloch functions are similar in both materials. If the $u_{v,k}(r)$ functions do not vary rapidly as a function of the wavevector k , the true wavefunction $\Psi_0(r,t)$ is related to the envelope function $\Psi(r,t)$ by

$$\Psi_0(r,t) \approx u_{v,k}(r)\Psi(r,t) \quad (3.9)$$

The useful effect of the envelope function approximation is to leave out the modulating effect of the rapidly varying $u_{v,k}(r)$ function while retaining the envelope $\Psi(r,t)$. Equation (3.8) can be solved separately inside any two adjacent layers and subjected to the continuity of $\Psi(r,t)$ and $\Psi'(r,t)/m^*(r)$ at the interface. These boundary conditions ensure current continuity at the heterointerface and are therefore physically justified [37,38,39].

Even in the absence of scattering ($U_S(r,t)=0$) there is, in general, no simple solution to equation (3.8) if $E_c(r,t)$ varies in all three dimensions and in time. If $E_c(r,t)$ is constant over some coordinates and in time, equation (3.8) admits plane wave solutions in these coordinates. In the case of interest, the potential profile varies in the z -direction but remains constant in the x and y directions and in time t ; the envelope function can therefore be written as

$$\Psi(r,t) = C\psi(z)e^{i(k_x x + k_y y)} e^{-iEt/\hbar} \quad (3.10)$$

which, by substitution into equation (3.8) yields

$$\frac{d^2 \psi}{dz^2} + \frac{2m^*}{\hbar^2} \epsilon(z)\psi(z) = 0 \quad (3.11)$$

where

$$\varepsilon(z) = E - E_c(z) - \frac{\hbar^2}{2m^*(z)}(k_x^2 + k_y^2) \quad (3.12)$$

The last term on the right hand side of equation (3.12) represents the in-plane dispersion relation of the quasi-two-dimensional electron gas. In order to decouple $\varepsilon(z)$ from its (x,y) dependence we follow Bastard [42] and set $(k_x, k_y) = (0,0)$ which will greatly simplify the calculation of the current density through the resonant tunneling device.

3.3 The Airy function method

In order to calculate the current density through a resonant tunneling device, one must first compute the transmission coefficient $T(E)$ through the double barrier as a function of energy and bias for all relevant energies. The transmission coefficient must then be calculated for several discrete energies; the energy mesh must be fine enough to represent all features of the $T(E)$ relationship. For non-trivial potential profiles, such as the double barrier in a constant electric field (see figure 3.1), the transmission coefficient can be calculated numerically by discretizing the potential into a fine mesh of constant potential steps each admitting a plane wave solution to the effective mass Schrodinger equation. The boundary conditions discussed in section 3.2 are then applied to every position mesh point. This solution method was followed by Vassel et al. [35]; clearly, it is computationally intensive since a finer position mesh must be used with an increasing electric field in order to minimize the discretization error associated with the step approximation to the linear potential profile. In order to avoid such heavy computation, an analytical solution for the transmission coefficient at a given energy using Airy functions, as used here, is attractive. The solution is still not fully analytical because the transmission coefficient must still be calculated for the energy mesh.

The analytical solution to Schrodinger's equation for a particle in a uniform electric field is known to be given in terms of Airy functions [45]. Airy functions have been used to describe a charged particle in a quantum

Figure 3.1 Step approximation to the linear potential profile.

Figure 3.2 Analytical solution using the Airy function.

well in presence of a uniform electric field [46] and have also been used to model resonant tunneling through double barrier single well structures [34,47]. In this work the approach followed by Xu [47] (transfer matrices instead of scattering matrices as in reference [34]) was chosen and extended to the case of tunneling through multiple well structures. For a one-dimensional, time independent, linear potential profile $E_c(z) = a - bz$, equation (3.11) becomes:

$$\frac{\delta^2 \psi}{\delta z^2} + \frac{2m^*}{\hbar^2} (E - a + bz) \psi = 0 \quad (3.13)$$

Letting $\phi = z/\gamma + \beta$, transforms equation (3.13) into

$$\frac{\delta^2 \psi}{\delta \phi^2} + \frac{2m^* \gamma^2}{\hbar^2} (E - a + \gamma b \phi + b \gamma \beta) \psi = 0 \quad (3.14)$$

Letting

$$\frac{2m^* \gamma^2}{\hbar^2} (E - a + \gamma b \phi + \beta \gamma b) = \phi \quad (3.15)$$

yields the so-called Airy differential equation [40]:

$$\frac{\delta^2 \psi}{\delta \phi^2} + \psi \phi = 0 \quad (3.16)$$

with

$$\gamma = \left\{ \frac{\hbar^2}{2m^* b} \right\}^{1/3} \quad (3.17)$$

and

$$\beta = \left\{ \frac{a \cdot E}{b \gamma} \right\} \quad (3.18)$$

A pair of linearly independent solutions to equation (3.16) are, by definition, $Ai(\phi)$ and $Bi(\phi)$, the Airy and complementary Airy functions respectively (some properties of $Ai(\phi)$ and $Bi(\phi)$ can be found in Appendix B). Hence the envelope function $\psi(z)$ in the j^{th} layer under a constant electric field is given by a linear combination of the Airy and complementary Airy functions

$$\psi_j(x) = CAi(\phi_j) + DBi(\phi_j) \quad (3.19)$$

where C and D are constants, in general complex numbers, determined by the boundary conditions. In detail, given the wavefunctions for the j^{th} and $(j+1)^{\text{th}}$ layers ψ_j and ψ_{j+1} , enforcing the continuity of ψ_j and ψ_{j+1} and of (ψ'_j/m_j^*) and of (ψ'_{j+1}/m_{j+1}^*) at the heterojunction yields the system of equations which needs to be solved in order to determine the constants. Here the prime denotes differentiation with respect to distance.

3.4 Transfer Matrix Formalism

As shown in section 3.3, the envelope function $\psi(z)$ is given by a linear combination of Airy functions in regions II, III and IV in figure 3.2. In regions 1 and 5 we let $\psi(z)$ be plane waves:

$$\psi_1(z) = e^{ik_z z} + R e^{-ik_z z} \quad (3.20a)$$

$$\psi_2(z) = C_1 Ai(\phi_2) + C_2 Bi(\phi_2) \quad (3.20b)$$

$$\psi_3(z) = C_3 Ai(\phi_3) + C_4 Bi(\phi_3) \quad (3.20c)$$

$$\psi_4(z) = C_5 Ai(\phi_4) + C_6 Bi(\phi_4) \quad (3.20d)$$

$$\psi_3(z) = S e^{ik_1 z} \quad (3.20e)$$

where the ϕ subscripts correspond to the respective regions in figure 3.2. The constants R , S and $C_1 - C_6$ are determined by the boundary conditions at the interfaces between the regions. Here the wavefunction in region I is assumed to be made up of a positive traveling plane wave of unity amplitude and a reflected wave of amplitude R while the wavefunction in region V consists of a single positive traveling plane wave with a wavevector k_L . The energy zero reference is taken as the emitter electrode conduction band edge in figure 3.2. The problem of calculating the constants can be transformed from a multiple boundary value problem into an initial value problem through the transfer matrix formalism as follows: enforcing the continuity of $\Psi(r,t)$ and $\Psi'(r,t)/m^*$ (where the prime denotes differentiation with respect to z) at $z=B$ for example, yields the following matrix equation

$$\begin{pmatrix} Ai(\phi_{12}) & Bi(\phi_{12}) \\ \alpha_1 Ai'(\phi_{12}) & \alpha_1 Bi'(\phi_{12}) \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} Ai(\phi_{21}) & Bi(\phi_{21}) \\ Ai'(\phi_{21}) & Bi'(\phi_{21}) \end{pmatrix} \begin{pmatrix} C_3 \\ C_4 \end{pmatrix} \quad (3.21)$$

Since from reference [40], p. 446, the Wronskian of $Ai(\theta)$ and $Bi(\theta)$, $W(Ai(\theta), Bi(\theta)) = \pi^{-1}$, solving for C_1 and C_2 produces

$$\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \frac{\pi}{\alpha_1} \begin{pmatrix} \alpha_1 Bi'(\phi_{12}) & -Bi(\phi_{12}) \\ -\alpha_1 Ai'(\phi_{12}) & Ai(\phi_{12}) \end{pmatrix} \begin{pmatrix} Ai(\phi_{21}) & Bi(\phi_{21}) \\ Ai'(\phi_{21}) & Bi'(\phi_{21}) \end{pmatrix} \begin{pmatrix} C_3 \\ C_4 \end{pmatrix} \quad (3.22)$$

Applying the same procedure at $z=B+W$ and $z=2B+W$ and cascading the resulting matrix equations yields an equation for S :

$$\begin{pmatrix} 1 \\ R \end{pmatrix} = \frac{i\pi^3}{2\alpha_0} \begin{pmatrix} -i\alpha_0 - 1 \\ -i\alpha_0 & 1 \end{pmatrix} \begin{pmatrix} \text{Ai}(\varphi_{11}) & \text{Bi}(\varphi_{11}) \\ \text{Ai}'(\varphi_{11}) & \text{Bi}'(\varphi_{11}) \end{pmatrix} \times$$

$$\begin{pmatrix} \text{Bi}'(\varphi_{12}) & \frac{-1}{\alpha_1} \text{Bi}(\varphi_{12}) \\ -\text{Ai}'(\varphi_{12}) & \frac{1}{\alpha_1} \text{Ai}(\varphi_{12}) \end{pmatrix} \begin{pmatrix} \text{Ai}(\varphi_{21}) & \text{Bi}(\varphi_{21}) \\ \text{Ai}'(\varphi_{21}) & \text{Bi}'(\varphi_{21}) \end{pmatrix} \times$$

$$\begin{pmatrix} \text{Bi}'(\varphi_{22}) & \frac{-1}{\alpha_2} \text{Bi}(\varphi_{22}) \\ -\text{Ai}'(\varphi_{22}) & \frac{1}{\alpha_2} \text{Ai}(\varphi_{22}) \end{pmatrix} \begin{pmatrix} \text{Ai}(\varphi_{31}) & \text{Bi}(\varphi_{31}) \\ \text{Ai}'(\varphi_{31}) & \text{Bi}'(\varphi_{31}) \end{pmatrix} \times$$

$$\begin{pmatrix} \text{Bi}'(\varphi_{32}) & \frac{-1}{\alpha_3} \text{Bi}(\varphi_{32}) \\ -\text{Ai}'(\varphi_{32}) & \frac{1}{\alpha_3} \text{Ai}(\varphi_{32}) \end{pmatrix} \begin{pmatrix} \text{Se}^{ikd} \\ i\text{Se}^{ikd} \end{pmatrix}$$

(3.23a)

with

$$\begin{aligned} \varphi_{11} &= \beta_1, & \varphi_{12} &= \frac{B}{\gamma_1} + \beta_1, \\ \varphi_{21} &= \frac{B}{\gamma_2} + \beta_2, & \varphi_{22} &= \frac{B+W}{\gamma_2} + \beta_2, \\ \varphi_{31} &= \frac{B+W}{\gamma_3} + \beta_3, & \varphi_{32} &= \frac{2B+W}{\gamma_3} + \beta_3, \end{aligned}$$

(3.23b)

and

$$\begin{aligned}\alpha_0 &= \frac{k_i m_1 \gamma_1}{m_1}, & \alpha_1 &= \frac{m_2 \gamma_2}{m_1 \gamma_1}, \\ \alpha_2 &= \frac{1}{\alpha_1}, & \alpha_3 &= \frac{m_2}{k_i m_1 \gamma_1},\end{aligned}\tag{3.23c}$$

where $d = 2B + W$, the thickness of the double barrier structure. Equation (3.23) is solved for S and the double barrier transmission coefficient is then obtained as

$$T = |S|^2 \frac{k_t}{k_i}\tag{3.24}$$

Although only the double barrier single quantum well case was discussed at any length in this section, the procedure used to calculate the transmission coefficient through a multiple quantum well structure is identical. The matrix equation corresponding to equation (3.23) increases in size but not in complexity and is easily handled with a computer yielding the appropriate T in equation (3.24).

3.5 Current Density Calculation

The current density through the resonant tunneling structure at a given bias voltage can be calculated by first computing the transmission coefficient as a function of energy $T(E)$, as discussed in the previous section and by then making use of the so-called Tsu-Esaki current density formula derived in reference [26]

$$J = \frac{m^* e k_B T}{2 h^3 \pi^2} \int_0^\infty T(E) D(E, E_F, T) dE\tag{3.25}$$

where $D(E, E_F, T)$ is the electron supply function

$$D(E, E_F, T) = \frac{1}{n} \left\{ \frac{1 + \exp[\beta(E_F - E)]}{1 + \exp[\beta(E_F - E - eV)]} \right\} \quad (3.26)$$

where E_F the Fermi level, E the incident electron energy, V the applied bias, e the electronic charge ($e=1.602 \times 10^{-19}$ C) and $\beta = 1/k_B T$ where $k_B = 1.3806 \times 10^{-23}$ J/K is Boltzmann's constant and T is the absolute temperature. The energy zero reference is defined at the emitting electrode conduction band edge.

The current density J is a sensitive function of the electrode Fermi level and, therefore, the latter must be determined as accurately as possible. In order to achieve high current densities, electrodes are usually heavily doped therefore necessitating the use of Fermi statistics when determining the Fermi level. The electrode Fermi level in the presence of donors (N_D) with an ionization energy E_D (below the conduction band edge) is calculated by numerically solving [41]

$$N_C F_{1/2} \left(\frac{E_F - E}{k_B T} \right) = \left\{ \frac{N_D}{1 + \delta \exp[\beta(E_D - E_F - E_D)]} \right\} \quad (3.27)$$

where $F_{1/2}(\eta)$ is the Fermi integral of order 1/2 of η , N_C is the electrode conduction band effective density of states and δ is the impurity level spin degeneracy. For GaAs electrodes doped with silicon donor atoms, $E_D = 5.8$ meV and $\delta = 2$ (spin up and spin down in the Γ band).

3.6 Numerical Implementation

The present model was implemented using double precision IBM FORTRAN VSFORT2.2 code. The Airy functions used in the calculation of the transmission coefficient were generated with the aid of the double precision I.M.S.L. standard mathematical functions libraries. Figure 3.3 illustrates the program flow for a general structure consisting of n wells and $n+1$ barriers.

The transfer matrix formalism discussed for the double barrier single well profile in section 3.4 was extended to the case of an arbitrary number n of wells and $n+1$ barriers supporting a uniform electric field. The extension is straightforward although quite tedious algebraically and is not included here because of space considerations. The source code for the present model is included in Appendix E. This version can handle an arbitrary number of wells each with a different thickness. Also, the first and last barrier heights may be chosen to be different from that of intermediate barriers although the actual barrier width is constant for all barriers.

The equilibrium Fermi level in the electrodes is calculated by solving equation (3.27) numerically by first considering a 1eV interval centered on the GaAs conduction band edge: the interval is then divided in one hundred equal segments and the segment for which equation (3.27) changes sign is known to contain the Fermi level solution. The procedure is repeated 10 times and therefore enables the user to know the Fermi level position at a given temperature and doping level within narrow error margin. In doing so, the Fermi integral of order 1/2 is approximated using the Aymerich-Humet [56] analytical expression for $\mathcal{F}_{1/2}(\eta)$ in order to speed up the solution by avoiding the evaluation of the improper integral found in the definition of $\mathcal{F}_{1/2}(\eta)$ (see Appendix C).

A typical program run begins with the initialization of variables (i.e. defining the variables as integer, real or complex numbers, reserving memory space for the arrays used for storing the transmission and reflection coefficients as a function of energy or the current density as a function of voltage) along with the definition of constants such as Planck's and Boltzman's constants. A bias voltage is then chosen; the electric field across the structure is then computed as the voltage divided by the total structure thickness. For a given applied bias, the transmission coefficient is computed as a function of energy using an arbitrarily assigned, sufficiently fine, energy mesh made up of equal energy intervals. Equation (3.25) is then evaluated using a simple trapezoidal integration algorithm to determine the current density J through the device. Although in principle, the integration is between 0 and infinite

energy, it was found that integrating from 0.0eV to 0.5eV is sufficient because of the weighting effect of the electron distribution function $D(E_F, E, T)$.

The number of energy steps for which the transmission coefficient is calculated depends on the actual structure and material system under consideration and must be determined through experimentation with the program until convergence from one run to the other is met. For instance, thick multibarrier structures, structures with high and thick potential barriers or material systems where the electron effective mass is large lead to very narrow resonance transmission peaks. Such narrow peaks are easily missed by the integration if it is not in "tune" with the structure under consideration; as a rule thicker structures require a finer integration mesh and the simulation therefore becomes more computer intensive as the thickness of the structure under consideration is increased.

Figure 3.3 Program flowchart for n-well structure.

Chapter Four

APPLICATION OF DEVICE MODELING

In this chapter we first illustrate, via examples, the application of the present model, as established in Chapter 3. In section 4.1, the behaviour of the transmission coefficient and of the current density integrand (see equation 3.25), through a biased double barrier resonant tunneling structure, is first examined as a function of the applied voltage. The I-V characteristic for that structure is then computed using the program written to implement the model discussed in Chapter 3. Further evidence pertaining to the validity of the Airy function method is also supplied by a comparison between the transmission coefficient of a double well structure, obtained with the aid of the present model, to numerically obtained results [35]. In the literature, there is little information regarding the use of Airy functions in the description of the electronic states in quantum wells and superlattices. Brennan [34], however, has considered Airy functions in his work on resonant tunneling. His results unfortunately show discrepancies when compared to the numerically calculated transmission coefficients by Vassel et al. [35] and therefore undermine the credibility of the Airy function method. Section 4.2 is used to reconcile analytical (through the use of Airy functions) and numerical results and in the process of doing so pinpoint for the first time the cause of the discrepancies found in Brennan's results.

4.1 Model use: Illustrative Examples

4.1.1 Single Quantum Well double Barrier

In order to demonstrate the validity of the present model, a double barrier structure previously considered by Brennan [34] and Vassel et al. [35] is used for illustrative purposes (see figure 4.1a). The resonant tunneling structure of interest consists of two 20Å $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers sandwiching a 50Å GaAs quantum well.

Figure 4.1 a) Single well structure considered in section 4.1.1 and b) double well structure of section 4.1.2.

For the simulation both the barriers and well regions were assumed to be undoped, the barrier height was taken to be 0.50eV while the electron effective mass in the well was taken as $m^*_{\text{GaAs}} = 0.067m_0$ and in the barriers $m^*_{\text{AlGaAs}} = 0.1087m_0$ respectively.

Figure 4.2 shows a plot of the transmission (T) and reflection (R) coefficients as a function of energy, on a linear scale, with 0.16V applied across the structure. Both $T(E)$ and $R(E)$ were evaluated separately to guard against possible errors; as expected $R+T=1$ (within a typically $\leq 2 \times 10^{-3}$ error margin due to truncation) for conservation of current probability density. The energy in transmission coefficient *versus* energy plots is always taken with respect to the emitter electrode conduction band edge. The narrow peaks in the transmission coefficient correspond to the energy of the quasi-stationary states of the 50Å GaAs quantum well. Figure 4.3 shows the evolution of the transmission coefficient as a function of energy with an increasing voltage applied across the structure. It can be seen from figure 4.3 that the transmission peaks move to lower energies with increasing bias. Specifically, transmission peaks are shifted to lower energies by an amount equal to 50% of the voltage applied across the double barrier structure. This is in complete agreement with the lowering of the quasibound states with respect to the emitter electrode conduction band edge as discussed in section 2.3. Even on resonance the transmission coefficient is not exactly equal to 1.0 because the perfect symmetry of the quantum well demanded by Fabry-Perot resonant tunneling is destroyed by the application of the electric field. The transmission coefficient shows some oscillations at energies greater than the barrier height. These oscillations are due to the resonance effects arising because of the presence of the continuum (or virtual) states of the quantum well. The results obtained here are in very close agreement with the ones obtained by Vassel et al. in reference [35]. Figure 4.4 represents the current density integrand of equation (3.25) and illustrates the weighting effect the distribution function $D(E, E_F, kT)$ has on the transmission coefficient plots of figure 4.3. Although the transmission coefficient is close to 1.0 for high energies the distribution function strongly suppresses the integrand at a few

Figure 4.2 Transmission (solid) and reflection (dashed) coefficient for the 20Å/50Å/20Å double barrier structure discussed in 4.1.1.

Figure 4.3 Effect of applied bias on the transmission coefficient dependence on energy. The applied voltages are 0.05V (solid), 0.16V (dotted) and 0.40V (dashed).

Figure 4.4 Current density integrand variation with applied bias.

Figure 4.5 Calculated I-V characteristic for the single quantum well double barrier of section 4.1.1.

electron volts above the emitter conduction band. The evaluation of equation (3.25) for twenty bias points, at 300°K, yields the I-V characteristic of figure 4.5. A Si doping density of $2 \times 10^{17} \text{cm}^{-3}$ was used; solving equation (3.27) numerically lead to a Fermi level of 31.8meV below the electrode conduction band edge. The integration of equation (3.25) was carried out using a constant energy mesh ($5 \times 10^{-4} \text{eV}$ steps) from 0.0eV to 0.5eV.

4.1.2 Double Quantum Well Structure

Vassel et al. [35] considered resonant tunneling through a structure made up of three equal height and equal barriers separated by two identical quantum wells. Taking the barrier height as 0.50eV, the barrier thicknesses as 20Å, the well widths as 50Å (with the electron effective mass equal to $m^*_{\text{GaAs}} = 0.067m_0$ in the wells and electrodes and $m^*_{\text{AlGaAs}} = 0.1087m_0$ in the barriers), they computed the transmission coefficient plots shown in figure 4.6. Physically, the splitting observed in the transmission peaks is due to the coupling between the quasistationary states belonging to the adjacent quantum wells. Figure 4.7 shows the results obtained via the Airy function method used in the present work, which are in excellent agreement with figure 4.6. The only noticeable difference resides in the fact that an Airy function solution may not be used at zero bias because the zero slope of the bands will cause γ and β to go to infinity (see equations (3.17) and (3.18)). However, the zero bias condition may be approximated by applying a very small (0.05V) bias across the structure.

4.2 Comparison to Previous [34] Airy Function Solution

As mentioned in the opening paragraph of this chapter, Brennan [34] explored the use of Airy functions in the description of electronic states in quantum wells and superlattices. As Brennan pointed out, the use of Airy functions leads to an exact, analytical solution for the transmission coefficient

Figure 4.6 Vassel's numerical results for the 2-well test structure of section 4.1.2 [35].

Figure 4.7 Analytical solution for the transmission coefficient for the 2-well structure at 0.05, 0.16 and 0.40V biases.

through a multiple barrier structure for a given incident electron energy. Given identical parameters as a starting point, both the analytical and the numerical (obtained by discretizing the potential profile as in figure 3.1) solutions should converge in order to be correct.

In reference [34], Brennan noted, without further explanation, that the transmission peaks corresponding to quantum well states appeared at consistently higher energies than those calculated by Vassel et al. [35] using the scheme of figure 3.1. The relative errors in the quasibound state energies were larger for the first states (ground state), sometimes reaching 233%, and reached 20-30% for the second bound state. These important discrepancies with Vassel et al.'s results [35] originate in the fact that Brennan did not enforce the continuity of the envelope function and of its derivative over the electron effective mass $\psi(z)/m^*(z)$ (as done in this work and in Vassel et al.[35]) but rather chose to use the continuity of the envelope function and of its derivative. As noted in Chapter 3, the latter set of boundary conditions does not conserve the probability current density defined as [45]

$$J = \frac{-i\hbar q}{2m(z)} \left\{ \psi \frac{d\psi^*}{dz} - \psi^* \frac{d\psi}{dz} \right\} \quad (4.1)$$

and is therefore physically incorrect in material systems involving a spatially modulated effective mass [37,38,39]. Figure 4.8 illustrates the impact of the enforcement of proper boundary conditions on the transmission coefficient as a function of energy: the continuous line was achieved by using the same boundary conditions as Brennan [34] while the dashed line is achieved through the present model.

Figure 4.8 Impact of proper boundary conditions. With Brennan's set of boundary conditions the transmission peaks with 0.16 bias occur at consistently higher energies (solid) than those given by the present model (dashed).

Chapter Five

RESONANT TUNNELING DEVICE DESIGN

This chapter centers on the design of GaAs/AlGaAs resonant tunneling structures using the model established in Chapter 3 and illustrated in Chapter 4. Experimental work on devices fabricated to these designs is reported in Chapter 6. First, the design of a simple double barrier single quantum well resonant tunneling diode is considered; since such a structure is symmetric about the quantum well, the I-V characteristic is expected to be very similar in both forward and reverse bias. The model is then used to design asymmetric, possibly rectifying, multiple quantum well resonant tunneling devices, which are expected to exhibit negative differential resistance only for the bias polarity defined as a forward bias.

The height of the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ conduction band barriers is assumed to be equal to 60% of the energy gap difference between GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ as discussed in Chapter 1. The conduction band electron effective mass in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ is taken to vary linearly with the aluminum mole fraction x as [44]:

$$m^*_{\Gamma}(x) = 0.067 + 0.083x \quad (5.1)$$

In line with the model presented in Chapter 3, the quantum well and barrier material is assumed to be undoped and therefore entirely supports the applied voltage, possible band bending in front of the emitter barrier and immediately following the collector barrier being neglected. The model could be modified to account for the difference in dielectric constant between the well and barrier regions but for the present purpose the permittivity is assumed to be constant and equal to that of GaAs ($13.1\epsilon_0$) throughout the structure, where ϵ_0 is the permittivity of free space.

5.1 Double Barrier Single Quantum Well Diode

The double barrier single quantum well diode is the simplest of all the resonant tunneling structures. In this case AlAs barriers were chosen for two

reasons: (i) AlAs provides the highest Γ -valley barriers ($\sim 1\text{eV}$) within the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ system and hence the use of AlAs barriers should enhance the off-resonance attenuation due to the double barrier system and therefore favor a high peak-to-valley current ratio; (ii) with AlAs being a binary compound, one intuitively expects more abrupt heterojunction interfaces between the GaAs material and the AlAs barriers than with a ternary alloy such as AlGaAs in the barriers. The well and barrier thicknesses were chosen as $40\text{\AA}$. A silicon dopant density of $N_D=2\times 10^{17}\text{ cm}^{-3}$ was selected near the barriers as a compromise between the need for high peak current density and for the need to prevent dopant migration from the electrode into the barrier and quantum well regions. Taking the electron effective masses as $m_{\text{AlAs}}^*=0.150m_0$ in the AlAs barriers and $m_{\text{GaAs}}^*=0.067m_0$ in the GaAs well yields $E_1=0.144\text{eV}$ for the first quasibound state in the well. The applied voltage for peak current is therefore expected to be equal to $2E_1/q=0.288\text{V}$.

5.2 Asymmetric Multiple Quantum Well Structures

5.2.1 Triple Well Asymmetric Resonant Tunneling Device

The designer of such nontrivial resonant tunneling structures must deal with a large parameter space as well as with the realistic limitations of the current epitaxial growth techniques, in this case Molecular Beam Epitaxy (MBE) [50]. As mentioned in Chapter 1, the physics of tunneling through mixed band heterojunctions is not well understood, so it is appropriate to restrict the aluminum mole fraction in the barriers to $x<0.45$ and insure that conduction band minimum has Γ symmetry throughout the structure. On the other hand, the barriers should be high enough to suppress the thermionic emission of electrons over the barriers. A value of $x=0.35$ was chosen as a compromise; the corresponding barrier is found from equation (1.1) to be equal to 0.27eV ($\sim 10kT$ at 300°K).

The multiple quantum well structure designed in this section incorporates 3 wells of varying thicknesses. As will become clear, it is crucial to the device operation that each grown layer thickness be close to its nominal

(designed) thickness. Assuming a GaAs growth rate of $1\mu\text{m/hr}$ ($2.78\text{\AA}/\text{sec}$ or approximately 1 monolayer/sec) and a shutter action time of 1sec it appears to be unreasonable to expect reliable growth of layers with a thickness smaller than $20\text{\AA}$. Furthermore, since the energy of the first quasibound state in each well needs to be adjusted independently, the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers should be thicker than 10 monolayers to prevent a strong coupling between the states belonging to adjacent wells. Arbitrarily we choose $42\text{\AA}$ (~ 15 monolayers) thick barriers. Much thicker barriers would provide a better wavefunction confinement within each well but to the cost of a lower transmission coefficient and hence lower current density through the structure.

Figure 5.1 shows the operation principle of the three-well, asymmetric, resonant tunneling device considered here: part a) shows the structure without bias while part b) illustrates the effect of an applied voltage. Three increasingly narrow quantum wells with $W_1 > W_2 > W_3$ are separated by identical barriers. The narrowing of the quantum wells causes their first quasibound state to be pushed to higher and higher energies $E_{1,1}^* < E_{1,2}^* < E_{1,3}^*$. In this case the energies $E_{1,n}^*$ are defined with respect to the bottom of the wells. (Recall that in infinitely deep quantum wells the energy eigenvalues are proportional to the square of the inverse well width, W^{-2}). Here the first subscript corresponds to the eigenstate and the second to the well in question. At zero bias the states are misaligned and no resonant tunneling current flow is possible through the structure. By raising the cathode band edge with the aid of a negative voltage (defined here as the forward bias condition) the three states are gradually brought into alignment with the emitter electrode conduction band edge bringing about an increase in the current flowing through the structure. The resonant tunneling current peaks when the three quasibound states are completely aligned. Any further increase in the applied voltage pulls the states out of their resonance condition thus quenching the resonant tunneling current, leading to a valley and negative differential resistance region in the forward bias I-V characteristic. Clearly, in the reverse bias condition, the applied voltage only contributes to pulling the quasibound states apart thus leaving a small leakage current unless higher states in adjacent wells come into alignment.

Figure 5.1 Operation principle of the 3 well asymmetric tunnel structure. On application of a positive bias the states align and allow a resonant tunneling current to flow. Upon negative bias, the states are pulled apart therefore quenching the tunneling current.

Quantitatively, the structure of figure 5.1 was designed by treating each well along with the associated barriers as a single double barrier single quantum well resonant tunneling diode and by insuring that the voltage drop across one barrier and the following well was equal to the first quasibound state energy eigenvalue in the next well when under the influence of the same electric field. In detail, assuming a voltage V_{a1} is applied to the widest well and two barriers, the structure supports an electric field F

$$F = V_{a1} / (2b + W_1) \quad (5.2)$$

where the barrier thickness is $b=42\text{\AA}$. W_1 must be chosen such that the energy of the first well, under a bias V_{a1} , aligns with the emitter electrode conduction band edge. Clearly, the first quasibound state eigenvalue for the second well, $E_{1,2}$, must be equal to (with respect to the pseudo-emitter A in figure 5.1 part b))

$$E_{1,2} = (b + W_1)F \quad (5.3)$$

defining

$$V_{a2} = (2b + W_2)F \quad (5.4)$$

a V_{a2} voltage drop across the second well and its two neighbouring barriers. The third quantum well width is determined in a similar way using the pseudo-emitter B in figure 5.1 part b). The energy renormalization and the use of pseudo-emitters is necessary because the energy levels of each well are determined by the peaks in the transmission coefficient *versus* energy plots produced with the present model and because, in this model, the energy zero reference is taken to be the emitter electrode. This method is easily extended to the n well case. Then, the energy of the first quasibound state belonging to the n^{th} well and the voltage across the n^{th} well and its two adjacent barriers are given by (for $n>1$)

$$E_{1,n} = ((n-1)b + \sum_{r=1}^{r=n-1} W_r)F \quad (5.5)$$

$$V_{an} = (2b + W_n)F \quad (5.6)$$

For n wells, the applied voltage for peak current (or resonance) is given by

$$V_{res} = \left((n+1)b + \sum_{r=1}^n W_r \right) F \quad (5.7)$$

Clearly, the present design methodology heavily relies upon the assumption of a uniform electric field over the well and barrier regions, as established in section 3.2.

For $x=0.35$ the barrier height is equal to 0.27eV, the electron effective mass is taken as $m_{\text{AlGaAs}}^* = 0.096m_0$ in the AlGaAs barriers and $m_{\text{GaAs}}^* = 0.067m_0$ in the GaAs electrode and quantum well regions. Keeping in mind that all layer thicknesses must be integer multiples of an atomic layer (about 2.83Å for both GaAs and AlGaAs) the following structure satisfies all the requirements enumerated thus far:

$$\begin{aligned} W_1 &= 84.90\text{\AA} \text{ (or 30 atomic layers),} \\ W_2 &= 50.94\text{\AA} \text{ (or 18 atomic layers),} \\ W_3 &= 36.79\text{\AA} \text{ (or 13 atomic layers),} \\ b &= 42.45\text{\AA} \text{ (or 15 atomic layers).} \end{aligned}$$

In the absence of an electric field, the first zero-bias quasibound state energies are, from the wider to the thinner well, $E_{1,1}^* = 0.0380\text{eV}$, $E_{1,2}^* = 0.0750\text{eV}$ and $E_{1,3}^* = 0.1072\text{eV}$ respectively. Following equation (5.7) the applied voltage for peak current in this structure is expected to be equal to $V_{res} = 0.129\text{V}$. Letting an asterisk (*) denote a zero field (i.e. flat band) quantity, the following relations are found to hold

$$E_{1,2}^* - E_{1,1}^* = \left(\frac{V_{a1} + V_{a2}}{2} \right) - bF \quad (5.8)$$

$$E_{1,3}^* - E_{1,2}^* = \left(\frac{V_{a2} + V_{a3}}{2} \right) - bF \quad (5.9)$$

relating the energy separation between the first quasibound states belonging to adjacent wells to the actual layer thicknesses. The tight alignment requirement for the quasibound states imposes tight growth constraints not only on the layer thicknesses but also on the aluminum content of the AlGaAs barriers since x determines the actual barrier height through equation (1.1). The calculated forward and reverse bias I-V characteristics for this structure, at 300°K appear in figure 5.2. As expected, the resonant tunneling current in the forward direction is much larger than in the reverse direction. The peak current density of 1750A/cm² occurs for an applied voltage of approximately 0.12V, in excellent agreement with the designed value. Some structure in the form of resonant peaks can be noticed for the reverse bias curve; these current peaks are due to the alignment of some higher states between adjacent wells and could be removed by using a design which incorporates thinner wells each containing a single quasibound state. No attempt is made here to determine which states come into alignment to produce these peaks.

5.2.2 Alternative Triple Well Continuum Tunneling Structure

The tight thickness control associated with the structure of figure 5.1 could be removed if tunneling were to occur through a band of continuum (also known as virtual) states that exist above the wells. If these virtual states were to be confined by barriers taller than the intermediate barriers, $eV_1 < eV_2$ (see figure 5.3a), negative differential resistance could be observed due to resonant tunneling through the virtual states belonging to the intermediate multiple quantum well structure. If the well width were decreased along the multiple quantum well stack, the associated virtual states should be raised (see figure 5.3b) causing a slanted virtual conduction band and therefore producing an asymmetric I-V characteristic. These structures, although more easily fabricated are more difficult to model; the modeling of this type of structure is beyond the scope of this thesis. However, an attempt was made to experimentally observe resonant tunneling through a slanted band of continuum states by replacing the two outermost AlGaAs barriers in figure 5.1 by taller (~1eV) AlAs barriers. The effect proposed here is entirely novel since resonant tunneling has yet to be achieved through "virtual states" and because the postulate of a slanted conduction band is new. Nakagawa et al. [69]

proposed and demonstrated [70] the so-called CHIRP (coherent hetero-interfaces for reflection and penetration) superlattice in which the superlattice period is gradually changed (both well and barrier thicknesses are allowed to vary in contrast to the well thickness only for the present device) to implement a slanted forbidden gap above the superlattice. The experimental I-V characteristic of the CHIRP superlattice displayed negative differential resistance only in one direction of current flow [70]. Potential benefits from structures such as those in figure 5.3 involve a decreased capacitance because of the structure thickness (increasing the electrode separation) as well as a reduction of the time an electron spends between the taller barriers because of the greater energy width of the continuum miniband (see Chapter 1).

The single and both triple well resonant tunneling structures (triple well and triple well with higher end barriers) discussed in this chapter were implemented by MBE with a Si doping density of $2 \times 10^{17} \text{ cm}^{-3}$ in the vicinity of the quantum well and barrier regions.

Figure 5.2 Calculated I-V characteristics for the triple well structure of section 5.2.1. Solid curve forward bias and dashed curve for reverse bias.

a) Symmetric continuum resonant tunneling device

b) Asymmetric continuum resonant tunneling device

Figure 5.3 a) Constant period multiple quantum well layer stack. Part b) illustrates the effect of grading the well widths upon the continuum states.

Chapter Six

EXPERIMENTAL WORK

6.1 Device Structures Investigated

The three resonant tunneling structures modeled and designed in chapter 5 were grown by Molecular Beam Epitaxy (MBE). The wafers were processed into top contacted mesa structures. All devices displayed the negative differential resistance associated with resonant tunneling through quantized states. The room and low temperature I-V characteristics were measured. In section 6.2 the device fabrication and processing is described, beginning with the MBE growth. This section also includes results of the analysis of the structures by Transmission Electron Microscopy (TEM) and Secondary Ion Mass Spectroscopy (SIMS); this material characterization provides valuable information in assessing the performance of the actual device structures *vis-a-vis* the modeling I-V characteristics for the nominal single and triple well structures presented in chapter 5. Section 6.3 presents the experimental results whilst section 6.4 discusses the device model developed here in the light of the experimental results.

6.2 Device Fabrication

6.2.1 Epitaxial Layer Growth

Three structures, MBE693-5, were grown in a VG Semicon V80H MBE system pumped down to a pressure of approximately $2.2 \times 10^{-5} \text{ Pa}$ ($1.65 \times 10^{-7} \text{ Torr}$). The substrate temperature was set at 630°C with an 8:1 As:Ga flux ratio: the GaAs growth rate was determined to be $1 \mu\text{m/hr}$ from previous calibration growth runs.

Figure 6.1 Epitaxial layers for MBE693.

Figure 6.2 Epitaxial layers for MBE694.

6.2.1.1 Single quantum well double barrier diode - MBE693

Figure 6.1 represents the layers grown. In detail, a 1000Å undoped GaAs buffer was first grown on a 3 inch diameter semi-insulating (Cr doped) GaAs substrate. A 10 period undoped superlattice buffer with each period consisting of a 25Å $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ barrier with a 25Å GaAs well was then grown to prevent the propagation of dislocations, originating from the substrate, into the epitaxial layers. The multiple quantum well buffer was followed by 2µm of n-type GaAs layer doped to $2 \times 10^{18} \text{ cm}^{-3}$ with Si and 0.1µm of n-type GaAs doped with Si to $2 \times 10^{17} \text{ cm}^{-3}$ forming the bottom electrode. The resonant tunneling structure itself was then made up of a 45Å undoped GaAs buffer to prevent dopant diffusion in the barrier/well region, a 40Å undoped AlAs barrier, a 40Å undoped GaAs quantum well, a second 40Å undoped AlAs barrier and another 45Å undoped buffer layer. The top electrode was made up of 0.1µm of n-type GaAs doped with Si to $2 \times 10^{17} \text{ cm}^{-3}$ followed by 0.5µm n-type GaAs doped to $2 \times 10^{18} \text{ cm}^{-3}$ with Si capped with a 100Å $\text{In}_y\text{Ga}_{1-y}\text{As}$ layer graded from $y=0.15$ to 0.5 with Si doping ramped from $2 \times 10^{18} \text{ cm}^{-3}$ to $2 \times 10^{19} \text{ cm}^{-3}$. The purpose of the InGaAs capping layer is to minimize the contact resistance because of the low Schottky barrier height associated with contacts to InAs (see Appendix D). Si was selected as the n-type dopant since it is characterized by a small activation energy (5.8meV below the GaAs conduction band edge) and because it has a very low diffusivity [50].

6.2.1.2 Triple Well Resonant Tunneling Devices - MBE694-5

Two different structures were made. Figure 6.2 shows the layers grown. In detail, a 4000Å GaAs buffer doped to $2 \times 10^{18} \text{ cm}^{-3}$ with Si was grown on a 3 inch diameter n^+ GaAs substrate of the same doping. The bottom electrode was also doped to $2 \times 10^{18} \text{ cm}^{-3}$ with the Si doping ramped down to $2 \times 10^{17} \text{ cm}^{-3}$ over 1000Å of GaAs. A 50Å undoped GaAs buffer was inserted between the heavily doped electrode and the multiple well structure. The multiple quantum well structure was kept undoped and was as follows: 42Å of $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ for MBE694, 85Å of GaAs, 42Å of $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$, 51Å of GaAs, 42Å of $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$, 37Å of GaAs and finally 42Å of $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ for MBE694. The structure for

MBE695 was almost identical to that of MBE694 with the exception being that the first and last $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ barriers were replaced by taller $42\text{\AA}$ AlAs barriers. The triple well structure was followed by a $50\text{\AA}$ undoped GaAs buffer layer. The top electrode then consisted of GaAs with Si doping ramped up from $2 \times 10^{17} \text{ cm}^{-3}$ to $2 \times 10^{18} \text{ cm}^{-3}$ over $1000\text{\AA}$, $4000\text{\AA}$ of Si doped GaAs at $2 \times 10^{18} \text{ cm}^{-3}$ and a $600\text{\AA}$ graded $\text{In}_y\text{Ga}_{1-y}\text{As}$ layer with $y=0$ to 0.5 with Si doping ramped up from $2 \times 10^{18} \text{ cm}^{-3}$ to $2 \times 10^{19} \text{ cm}^{-3}$.

6.2.2 Structural Analysis

6.2.2.1 TEM Measurements

High magnification TEM photographs were taken in order to assess the crystal quality of the epitaxial layers as well as to determine the actual thickness of the various epitaxial layers. (Since TEM measurements only detect compositional changes from one layer to another, TEM is unsuitable to determine the dopant distribution in the devices. SIMS measurements were used to chart out the Si dopant profile throughout the resonant tunneling devices).

Figure 6.3 (891373) shows the multiple quantum well superlattice buffer grown close to the semi-insulating substrate on MBE693. Figure 6.4 (891286) is a shot of the double barrier resonant tunneling structure of section 6.2.1.1 with a magnification factor of $500,000\times$. Normally, the thickness of each layer should be equal to $40\text{\AA}$. The actual layer thicknesses measured from figure 6.4 (and other similar photographs) are found to fluctuate between 30 and $40\text{\AA}$ for the AlAs barrier closest to the substrate, between 40 to $54\text{\AA}$ for the GaAs quantum well and between 30 to $40\text{\AA}$ for the topmost AlAs barrier (all measurements are within a $\pm 7\text{-}12\%$ error margin). Closer inspection of figure 6.4 reveals some interface roughness at the junction between epitaxial layers. The interface roughness could be due to interdiffusion or alloying, at the hetero-interface, which might have been brought about by the relatively high ($1\mu\text{m/hr}$) growth rate. More abrupt interfaces could have been achieved

Figure 6.3 TEM photograph of MQW buffer in MBE693.

Figure 6.4 Double barrier structure magnified
500,000x times.

Figure 6.5 Graded InGaAs capping layer -MBE693.

with a lower growth rate ($0.5\mu\text{m/hr}$) when used in conjunction with an interruption of growth at each interface, followed by an annealing cycle (to allow each atom to reach its proper lattice position) before commencing the the growth of the next layer. Figure 6.5 (891277) is a photograph of the graded $\text{In}_y\text{Ga}_{1-y}\text{As}$ capping layer. The interface between InGaAs and GaAs is rich in microstructural defects associated with the strain due to the large lattice mismatch ($\Delta a/a_0 \times 100\% = 7.16\%$ implying that roughly one atom out of 14 is misplaced at the interface) between GaAs and InAs .

Figure 6.6 (891459) is a TEM photograph of the 3-well resonant tunneling structure of section 6.2.1.2, labeled MBE694. Interfaces appear to be abrupt and defect free. The poor contrast between the layers is due to the low Al concentration in the barriers (35%). The barrier layer widths are, from the substrate up, 48, 44, 44 and $44\text{\AA}$ with a $\pm 10\%$ relative error. The well widths are $W_1=88\text{\AA}$ (to $\pm 7.3\%$), $W_2=56\text{\AA}$ ($\pm 8.6\%$) and $W_3=36\text{\AA}$ ($\pm 10.5\%$). Figure 6.7 (891354) is a dark field image of MBE695 showing the two outermost AlAs barriers at a higher contrast. From this photograph, the layer thicknesses can be determined to be equal to (from the substrate up, for the barriers) 48, 48, 44 and $40\text{\AA}$ within $\pm 10\%$. The well widths are found to be $W_1=92\text{\AA}$ (to $\pm 7.2\%$), $W_2=54\text{\AA}$ ($\pm 8.7\%$) and $W_3=40\text{\AA}$ ($\pm 10\%$). (Relative errors quoted for dimensions are due to the combination of a $\pm 5\%$ magnification error range on the electron microscope and of the reading error). Figure 6.8 is a lattice image of MBE695; the GaAs/AlAs interfaces appear to be rough, almost corrugated. With the aid of figure 6.2 it is readily verified that there is good agreement between the nominal and experimental layer thicknesses. The typical thickness deviations are equal to approximately two monolayers ($\sim 6\text{\AA}$) per layer, indicating the type of thickness control available in MBE.

6.2.2.2 SIMS Analysis

A SIMS analysis was carried out for MBE693-5 in order to obtain the Si, Al, In and Ga profiles throughout the layers. Structures of the order of $100\text{\AA}$ or less (such as GaAs quantum wells or AlGaAs barriers) cannot be resolved in SIMS profiles. However, the presence of Al in barrier regions shows up as Al

Figure 6.6 Triple well resonant tunneling structure MBE694.

Figure 6.7 Triple well structure MBE695.

Figure 6.8 Lattice image of MBE695 showing the interface roughness.

2

OF/DE

2

Micro

spikes in a SIMS profile. Therefore, the SIMS profiles in this section provide information on the Si dopant distribution in relation to the AlGaAs barrier position as well as to the InGaAs capping layer.

Figure 6.9 is the SIMS profile of the double barrier resonant tunneling diode MBE693. As expected from the MBE growth parameters, the InGaAs capping layer is about 100Å thick with a Si doping density approaching 10^{19}cm^{-3} . However, the actual electrode doping determined from the SIMS analysis is found to be approximately equal to 10^{18}cm^{-3} while the 10^{17}cm^{-3} region on the substrate side is somewhat thicker than 1000Å. This asymmetry in the doping profile close to the double barrier structure is expected to account for some asymmetry in the device I-V characteristic. According to figure 6.9, the Si trace increases, rather than falling effectively to zero, within the quantum well region. This spike, rather than being due to a rise in the Si concentration, is an interference effect: indeed, some Al atoms are mistaken for Si atoms by the quadrupole mass analyzer (recall that Al and Si are atomic numbers 13 and 14 respectively in the periodic table of elements).

Figure 6.10 and 6.11 show the SIMS profiles obtained for MBE694 and MBE695 respectively. First consider MBE694. Starting from the n^+ GaAs substrate at approximately $1.25\mu\text{m}$ from the surface we note a drop in the Si concentration due to the outdiffusion from the substrate into the initially undoped GaAs growth. The Si doping is then ramped up to 10^{18}cm^{-3} . At about $0.8\mu\text{m}$ from the surface the Si concentration is ramped down to 10^{17}cm^{-3} over 1000Å. The Al spike indicates the presence of the nominally undoped 3-well structure. Doping is then ramped up from 10^{17}cm^{-3} to 10^{18}cm^{-3} over 500Å and kept constant at that level for 4000Å before an approximately 500Å thick heavily doped ($\text{Si } 2 \times 10^{19} \text{ cm}^{-3}$) InGaAs capping layer is reached. MBE695 is very similar with the exception of lower doping levels ($6 \times 10^{17}\text{cm}^{-3}$) in what should be heavily doped (nominally $2 \times 10^{18}\text{cm}^{-3}$) electrodes. This low dopant concentration may be attributed to the depletion of the Si source over many growth runs.

Figure 6.9 SIMS profile for the double barrier single well structure labeled MBE693.

Figure 6.10 SIMS profile for the triple barrier double well structure labeled MBE694.

Figure 6.11 SIMS profile for the triple barrier double well structure labeled MBE695.

6.2.3 Device Processing

The epitaxial layers were processed into top contacted 2 terminal devices using a standard post-and-bridge mask set. Following an initial wafer cleaning step, a mesa was etched (0.8 - 1 μ m deep for MBE693 and 0.7-0.9 μ m deep for MBE694-5). The mesa diameters were 5, 10, 20 and 25 μ m. A ring contact to the bottom electrode was formed by Ni/GeAu evaporation and lift-off followed by a rapid thermal annealing cycle of 15sec at 415°C in a H₂/N₂ ambient. A 2200Å SiO₂ blanket was then sputter deposited and a contact window to the top electrode was opened through the SiO₂ layer with a 20sec wet etch in a 1:1 HF:H₂O solution. Non-alloyed top contacts to the mesas were formed by Ti/Pt/Au evaporation [49]. Figures 6.12 and 6.13 show a plan and cross sectional view of the structures.

6.3 Experimental I-V Characteristics

Current-voltage measurements were made on all three resonant tunneling structures with the aid of an HP4145B semiconductor parameter analyzer. I-V characteristics were obtained, in the dark and at different temperatures by placing the devices within a MMR Technologies Low Temperature Probing station equipped with a K-20 programmable temperature controller run by an HP9000 microcomputer. The semiconductor parameter analyzer was operated in a voltage driven mode that is, it applied a voltage across the devices and measured the resulting current. The three structures, MBE693-5, consistently displayed the negative differential resistance region associated with resonant tunneling.

6.3.1 Single Well Resonant Tunneling Diode - MBE693

Figure 6.14 shows typical I-V characteristic of a 10 μ m diameter mesa at 100°K and 200°K. The positive voltage range in figure 6.14 corresponds to an electron flow from the substrate up into the top electrode. It was found that the current density was approximately equal for different size mesas. No

Figure 6.12 Plan view of device contacting.

Figure 6.13 Idealized process cross-section.

negative differential resistance was apparent at room temperature although a valley in the I-V characteristics appeared when the devices were cooled down below 230°K. The low peak-to-valley ratio at high temperatures (1 at 230°K and 2.31 at 100°K) and low peak current density of 242A/cm² at 230°K (187A/cm² at 100°K) are attributed to the interface roughness at the barriers as shown by the TEM photograph in figure 6.4. The asymmetry in the peak current voltage between forward and reverse bias is consistent with the asymmetric Si distribution around the barriers as shown in figure 6.9. Figure 6.15 is a plot of the peak and valley currents, in the forward bias regime, as a function of inverse temperature. It can be seen that although the peak current density nearly remains constant the valley current density steadily decreases as temperature decreases (1/kT increases).

6.3.2 Triple well asymmetric devices MBE694-5

6.3.2.1 MBE694

I-V characteristics for MBE694 displayed a negative differential resistance region for temperatures up to 350°K. Figure 6.16 displays typical I-V plots for temperatures of 80°K and 300°K for a 10μm diameter mesa. The peak-to-valley ratio was typically 1.3 at 300°K and 4.0 at 80°K. To the best of the author's knowledge, this is the first demonstration of resonant tunneling through a triple-well structure at room temperature. Furthermore, the high peak current density of 8600A/cm² at 300°K (10000A/cm² at 80°K) for these devices is probably the highest ever achieved to this date for multiple well structures of this thickness. The author has recently become aware that Summers et al. [65] independently developed similar devices. In comparison, however, Summers et al. did not demonstrate negative differential above 200°K and showed a maximum current density of approximately 3000A/cm².

Figure 6.16 clearly shows that a strong resonant tunneling current only flows from the substrate up; that is, in the forward bias case as defined in section 5.2. Closer examination of the reverse bias low temperature

***** GRAPHICS PLOT *****
RT693 200/100K 10 μ m

Figure 6.14 Typical I-V characteristic of 10 μ m diameter mesa for the single well sample MBE693 at 100°K and 200°K.

Figure 6.15 Peak (+) and valley (Δ) density as function of inverse temperature for the single well structure MBE693.

characteristic (80°K) shows that resonant tunneling current does actually flow, giving rise to a small region of negative differential resistance. This resonant tunneling current must be attributed to a resonance condition involving the second state in the wider well (W_1) and most likely the second state of the central well (W_2).

Figure 6.17 is a plot of the natural logarithm of the peak and valley current (in mA) densities as a function of inverse temperature, $1/kT$. The peak current density remains more or less constant over the whole temperature range while the valley current density decreases steadily. Between 200°K and 350°K the valley current appears to decrease exponentially following an Arrhenius-type law indicating that the valley current might be the result of an activated process. As the temperature is decreased from 200°K to 100°K the valley current density saturates therefore hinting that two separate processes might be involved in controlling the valley current. The valley current density data can be fitted to a straight line with a slope of -38meV and with a high correlation coefficient ($r \geq 0.995$) between 200-350°K. The LO optical phonon effective energy in AlGaAs is known to be equal to 38 meV [72] and is not expected to change very much as a function of temperature (the GaAs LO phonon energy changes by 0.011meV between 80°K and 350°K [67]). Mendez et al. [57] have given strong experimental evidence that the valley current in AlAs-GaAs-AlAs resonant tunneling diodes is controlled by the Γ -X valley separation between the well (and electrode material) and the barrier respectively. In their experiment, they have shown that the current peak-to-valley ratio is decreased with the application of hydrostatic pressure; although the Γ - Γ valley separation remains approximately constant, the Γ -X separation between the well and barrier material decreases at a rate of -12meV/kbar. Clearly then, as the Γ -X valley separation decreases, more electrons may scatter (via phonons, impurities or surface roughness) into the X band and therefore allow a higher valley current to flow. The actual band transfer mechanism is yet unknown but the data presented in figure 6.18 raises the possibility that, at least above 200°K, the band transfer mechanism might be due to phonon-assisted tunneling by absorption of an optical phonon with an energy of 38meV.

***** GRAPHICS PLOT *****
RT693 300K/80K 10 μ m

Figure 6.16 Typical I-V characteristics for a 10 μ m diameter mesa for the triple well sample MBE694 at 80°K and 300°K.

Figure 6.17 Peak (+) and valley (Δ) density as function of inverse temperature. The range covers 100°K to 350°K. The straight line has a slope of -38meV (the optical phonon energy in AlGaAs).

***** GRAPHICS PLOT *****
RT695 80K 10 μ m

Figure 6.18 Typical I-V characteristics for a 10 μ m diameter mesa for the triple well sample MBE695 at 80°K.

6.3.2.2 MBE695

MBE695 did not show any negative differential resistance at room temperature. In this case, the structures had to be cooled below 200°K before negative resistance was seen. Figure 6.18 shows typical characteristics for 10 μ m devices at 80°K. The forward peak-to-valley ratio was 2.0 with $J_p=43\text{ A/cm}^2$. A very weak negative differential resistance is present in the reverse bias regime (positive voltages in figure 6.19) although a much stronger one is present under forward bias. The generally poor performance at high temperatures is easily explained in terms of the interface roughness present at the interfaces between the AlAs barriers and GaAs as displayed in figure 6.8. The interface roughness modifies the potential profile of the barriers in an unpredictable ways and introduces scattering which destroys the phase coherence needed for Fabry-Perot-like tunneling. The low peak current density measured for MBE695 is due, in major part, to the low Si doping in the electrodes as was shown in figure 6.11.

6.4 Discussion: Comparison to Model Predictions

6.4.1 Single well resonant tunneling diode (MBE693)

A comparison between the theoretical curve of figure 5.1 and the experimental curve of figure 6.14 produces several significant differences. First, the experimental I-V characteristic is not symmetrical for forward and reverse biases because of the asymmetrical Si dopant profile about the quantum well which was already pointed out in section 6.2.2.2. Furthermore, the experimental peak current voltage, $V_{pexp} \sim 1.2\text{V}$ is greater than the theoretical value of $V_{pth} \sim 0.30\text{V}$. The discrepancy in the peak current voltage is believed to be due to the presence of accumulation and depletion layers in the emitter and collector electrodes respectively and to possible ohmic losses in the contacts to the device. Another factor contributing to the discrepancy in V_p is the presence of the undoped buffer layers near the well and barrier regions and the fact that the well and barriers are kept undoped; under thermal equilibrium, the Fermi levels line up throughout the device and the

quantum well region is raised by an amount ΔV with respect to the electrode conduction band edge necessitating the application of an extra ΔV in order to reach the resonance condition. Moreover, no allowances are made here to account for the effect of possible interface states present at the electrode/barrier or well/barrier interfaces on the peak current voltage.

The present model grossly underestimates the valley current flowing in real devices apparently indicating that the excess current is due to some non-resonant transport process through other bands - in all likelihood through the X band for resonant tunneling diodes implemented in the AlGaAs/GaAs material system [57]. The actual barrier thickness was found from the TEM measurements, in section 6.2.2.1, to fluctuate between 30 and 40Å. Thinner barriers lead to broader transmission peaks (see figure 2.4) and therefore allow a higher current density to flow through the quantum well (of course, the transmission through the narrower barriers would dominate). Also, the electron accumulation layer present in front of the emitting barrier contributes to raise the Fermi level with respect to the conduction band edge; the actual Fermi level for the emitting electrode used in the computation should therefore be higher than that of the electrode under thermal equilibrium (31meV below the conduction band edge for a Si concentration of $2 \times 10^{17} \text{cm}^{-3}$ at 300°K). A simulation run with a 40Å well with 30Å barriers along with a Fermi level located 31meV below the conduction band edge in the emitter produces a peak current density of approximately 100A/cm² at 300°K, still short of the 242A/cm² obtained experimentally. A similar run but this time with the Fermi level set to 1meV above the emitter conduction band edge produces a peak current density of 286A/cm² at 300°K, in much better agreement with the experimental results. Figure 6.19 illustrates the results of these simulation runs. The data were smoothed to get rid of a ripple in the I-V curve, an artifact introduced by the integration of extremely narrow peaks in the transmission coefficient arising because of the very low transmission coefficient for an individual AlAs barrier of this thickness.

Figure 6.19 Calculated I-V characteristics at 300°K with 30Å barriers for MBE693. Fermi levels of -31meV (solid) and 1meV (dashed) with respect to the emitter conduction band edge.

6.4.2 Triple well device (MBE694)

Here again, the experimental peak current voltage in the forward bias regime ($V_{pexp} \sim 1.2V$) is greater than that predicted by the model ($V_{pth} \sim 0.13V$) for the same reasons as discussed above for the single well device: band bending in the electrodes contributes to push the current peak to higher voltages by screening the electric field applied to the quantum well and barrier regions. The experimental valley current is still larger than that expected from the present model because non-resonant current components are not accounted for. The experimental peak current density $J_p = 8600 A/cm^2$, is greater than the one predicted by the model in figure 5.3 ($1776 A/cm^2$ with $E_F = -31 meV$ below the emitter conduction band edge). In this case the actual layer thicknesses are quite close to the designed values as verified from TEM measurements for MBE694 in section 6.2.2.1. Figure 6.20 shows the I-V characteristics produced by a simulation of the nominal structure of section 5.2.1 while taking the Fermi level to be 10meV and 15meV above the emitter electrode conduction band edge to take into account the effect of the electron accumulation region in front of the barrier in the emitting electrode. For these Fermi levels, the calculated peak current densities reach $6667 A/cm^2$ and $7634 A/cm^2$ respectively, in much better agreement with the experimental value.

Figure 6.20 Calculated forward I-V characteristic for MBE694 with adjusted parameters at 300°K. Fermi levels of 10meV (dashed) and 15meV with respect to the emitter conduction band edge.

Chapter Seven

CONCLUSION AND FUTURE WORK

Modeling

The model developed in this work has been shown to account for the major features of the I-V characteristics of single and multiple well two-terminal resonant tunneling devices. The application of the present model in the analysis and design of a novel class of asymmetric resonant tunneling devices and the success met in the actual device implementation establish the model as a good first order analysis and design tool for resonant tunneling devices incorporating undoped (or unintentionally doped) quantum well and barrier regions.

When compared to the experimental I-V curves, the model characteristics showed discrepancies in the peak current voltage V_p and in the peak current density J_p . In both cases, the errors have been explained to be due to band bending in the electrodes in the form of an accumulation layer at the emitting electrode barrier and depletion layer immediately following the collector barrier. With proper corrections made to the simulation parameters, the present model correctly reproduced the experimental peak current densities for the single and triple well resonant tunneling devices MBE693 and MBE694 respectively. The discrepancies in V_p and in J_p indicate the importance of the inclusion the self-consistent solution of Schrodinger's and Poisson's equations in order to achieve a more accurate theoretical estimate of V_p and J_p . The present model was found to overestimate the valley current density for both single and triple well resonant tunneling devices. This over-estimate is believed to be due to over-idealization in the form of the zero scattering approximation, of the single band approximation and of the abrupt heterojunction approximation.

Future modeling work should focus on the inclusion of self-consistency effects together with the effect of scattering events on the tunneling process, effect of other bands and the relaxation of the conservation of momentum

parallel to the interface $p \parallel (p_x, p_y)$ since solid state junctions are in general not planar.

Experimental work

Single well and triple well tunneling structures, designed with the aid of the present model, were successfully demonstrated. Negative differential resistance in a single well double barrier diode was observed below 230°K. Room temperature negative differential resistance was demonstrated in asymmetric triple well structures with $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ barriers. A similar structure was grown but with AlAs end barriers in an attempt to observe resonant tunneling through virtual states above the multiple quantum well stack. The structure did show negative differential resistance associated with tunneling through its bound states but only at low temperatures because of a low doping density in the electrodes and of the poor morphology of the GaAs/AlAs interfaces.

The temperature dependence of the peak and valley current densities was studied in both single well (MBE693) and triple well (MBE694) structures. The peak current density was shown to remain approximately constant with decreasing temperature while the valley current density decreased steadily with decreasing temperature in both cases. The valley current density in MBE694 exhibited an exponential dependence on inverse temperature with an activation energy equal to 38meV over the temperature range 200°K to 350°K. These data, together with the results found in reference [57], suggest that the valley current over that temperature range is phonon-assisted and requires the absorption of a 38meV optical phonon for momentum conservation for the transfer of the tunneling electron from the Γ band to the X-band.

Further experimental work should aim to determine if the valley current dependence on inverse temperature in resonant tunneling devices implemented in material systems other than AlGaAs/GaAs also exhibits an activation energy equal to the optical phonon energy of the given system. Furthermore, attempts should be made to observe negative differential resistance associated with resonant tunneling through virtual states. With

this in mind, another choice of material system could be favourable. Indeed, a structure with $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ end barriers and deep (below the GaAs emitter conduction band edge) pseudomorphic $\text{In}_x\text{Ga}_{1-x}\text{As}$ wells separated by GaAs barriers appears to be a good candidate since in this case, the virtual states band would appear slightly above the intermediate GaAs barriers and therefore be readily accessible to the incident electron distribution in the emitter electrode.

APPENDIX A

Energy gap and lattice constant variation in III-V Compounds

Figure A.1 Energy gap and lattice constant variation with composition for III-V compounds. A solid line indicates that the energy gap is direct while the dashed line indicates that the energy gap is indirect [50].

APPENDIX B

Some properties of the Airy functions

By definition, the Airy and complementary Airy functions, $Ai(z)$ and $Bi(z)$ respectively, are a pair of linearly independent solutions of the so-called Airy differential equation [40]

$$\frac{d^2 w}{dx^2} - xw = 0 \quad (B.1)$$

The Airy functions can be represented in terms of the Bessel $J_\nu(\zeta)$ and of the modified Bessel functions of order ν , $K_\nu(\zeta)$ and $I_\nu(\zeta)$ with the following change of variables [40]

$$\zeta = \frac{2}{3}x^{3/2} \quad (B.2)$$

Then,

$$Ai(x) = \frac{1}{3}\sqrt{x} [I_{-1/3}(\zeta) - I_{1/3}(\zeta)] = \frac{1}{\pi}\sqrt{x/3} K_{1/3}(\zeta) \quad (B.3)$$

$$Ai(-x) = \frac{1}{3}\sqrt{x} [J_{1/3}(\zeta) + J_{-1/3}(\zeta)] \quad (B.4)$$

$$Bi(x) = \sqrt{x/3} [I_{-1/3}(\zeta) + I_{1/3}(\zeta)] \quad (B.5)$$

$$Bi(-x) = \sqrt{x/3} [J_{-1/3}(\zeta) - J_{1/3}(\zeta)] \quad (B.6)$$

Figure B.1 is a plot of the $Ai(x)$ and $Bi(x)$ for $-10 < x < 5$. Further properties of the Airy functions can be found in reference [40].

Figure B.1 $Ai(x)$ solid curve, $Bi(x)$ dashed curve.

APPENDIX C

Aymerich-Humet Approximation to $F_{1/2}(\eta)$

The Fermi integral of order 1/2 must be evaluated when dealing with degenerately doped semiconductors, that is, when the Fermi level approaches or exceeds the band edges. By the definition the Fermi integral of order 1/2 is given by

$$F_{1/2}(\eta) = \frac{1}{\Gamma(3/2)} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{1 + \exp(\varepsilon - \eta)} \quad (C.1)$$

where $\Gamma(x)$ is the Gamma function, $\eta = (E_F - E_C)/kT$ is the reduced Fermi energy and $\varepsilon = (E - E_C)/kT$ is a suitable dimensionless energy variable. Equation (C.1) may be approximated by [56]

$$F_{1/2}(\eta) \approx \frac{1}{e^{-\eta} + 3\sqrt{\pi/2} [(\eta + 2.13) + (|\eta - 2.13|^{2.4} + 9.6)^{5/12 - 3/2}]} \quad (C.2)$$

valid for any η . As seen in figure C.1, the relative error between the value calculated by (C.2) and the real value of equation (C.1) oscillates several times in sign but the maximum error excursions of $F_{1/2}(\eta)$ barely exceed 0.5%.

Figure C.1) Maximum relative error in (C.2), curve $j=1/2$ [56].

APPENDIX D

Ohmic Contacts to Compositionally Graded $\text{In}_x\text{Ga}_{1-x}\text{As}$ Layers

Low resistance ohmic contacts to n-type GaAs are difficult to achieve because of a $\sim 0.8\text{eV}$ Schottky barrier associated with the metal-GaAs interface. Figure D.1 part a) represents the energy band diagram for the metal/n-GaAs contact. It has been found experimentally that the barrier height to GaAs is more or less independent of the actual metal used and is roughly equal to 0.8eV . This effect is believed to be due to an abundance of mid gap states at the interface between the metal and the GaAs surface. The metal Fermi level is therefore said to be pinned in the center of the GaAs forbidden gap.

On the other hand, InAs surfaces exhibit Fermi level pinning in the conduction band. The situation for a metal/n-InAs contact is shown in part b) of figure D.1: in this case the contact is ideal since the Schottky barrier height $\phi_b \leq 0$. Part c) shows that if an InAs layer is inserted between the metal and the GaAs surface the contact behaves as a simple metal/n-GaAs contact because of the large conduction band discontinuity at the InAs/GaAs heterojunction. Woodall et al. pointed out that if, however, the InGaAs layer is graded (by grading the In mole fraction in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloy) as shown in figure D.1 part d), there is no conduction band discontinuity and a good ohmic contact is obtained when the metal is deposited over the InGaAs graded layer.

Nittono et al. [49] have demonstrated extremely low contact specific resistance ($\rho_c = 5 \times 10^{-8} \Omega\text{cm}^2$) with a $600\text{\AA}$ graded region with $x=0-0.65$ and with a carrier concentration of $1.5 \times 10^{19}\text{cm}^{-3}$ and Ti/Pt/Au metal layers ($200/200/4000\text{\AA}$).

Figure D.1 Energy band diagrams for ohmic contacts to n-type GaAs.

APPENDIX E

Program Source Code

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```

C ----- THE00010
C THIS PROGRAM COMPUTES THE CURRENT DENSITY THROUGH MULTIPLE THE00020
C WELL RESONANT TUNNELING STRUCTURES USING AIRY FUNCTIONS IN AN THE00030
C ENVELOPE FUNCTION APPROXIMATION. THE00040
C THE00050
C EACH WELL WIDTH MAY BE SPECIFIED INDIVIDUALLY AND THE END THE00060
C BARRIERS MAY BE HIGHER THAN THE INTERMEDIATE BARRIERS. THE THE00070
C BOUNDARY CONDITIONS USED AT EACH INTERFACE ENSURE THE THE00080
C CONSERVATION OF CURRENT DENSITY. THE00090
C ----- THE00100
C • DOUBLE PRECISION • THE00110
C THE00120
C IMPLICIT DOUBLE PRECISION (A-H,L-Z) THE00130
C REAL*8 MO,KI,KT,SWDTH(10),ENERGY(99999),TRANS(99999),K,KTT THE00140
C REAL*4 JC(50),VOLT(50) THE00150
C COMPLEX*16 S,R THE00160
C INTEGER NIV,NWELLS THE00170
C THE00180
C THE00190
C THE00200
C ----- THE00210
C DEFINITIONS THE00220
C ----- THE00230
C H = PLANCK'S CONSTANT THE00240
C HBAR = REDUCED VALUE OF PLANCK'S CONSTANT THE00250
C MO = FREE ELECTRON MASS THE00260
C E = ELECTRON CHARGE THE00270
C ENRGV = ELECTRON ENERGY IN SWEEP THE00280
C BARH = BARRIER HEIGHT IN ELECTRON VOLTS THE00290
C BARW = BARRIER WIDTH IN ANGSTROMS THE00300
C WELW = WELL WIDTH IN ANGSTROMS THE00310
C WEFM = EFFECTIVE MASS IN WELL MATERIAL /MO. THE00320
C BEFM = EFFECTIVE MASS IN BARRIER MATERIAL /MO. THE00330
C ANG = 1 ANGSTROM (10E-10 METER). THE00340
C DE = ENERGY INCREMENT THE00350
C TEMP = TEMPERATURE IN DEGREES KELVIN. THE00360
C THICK = SAMPLE THICKNESS (ANG.) THE00370
C BIAS = APPLIED VOLTAGE (DROPPED ENTIRELY ACROSS RTD) THE00380
C SLOPE = BIAS/THICK THE00390
C SUBARH = SUPERLATTICE BARRIER HEIGHT THE00400
C SUBARW = SUPERLATTICE BARRIER WIDTH: CONSTANT THE00410
C SWDTH = SUPERLATTICE WELL WIDTH ARRAY OF DIMENSION "NWELLS" THE00420
C NWELLS = TOTAL NUMBER OF WELLS IN STRUCTURE THE00430
C THE00440
C THE00450
C ----- THE00460
C CONSTANT VALUES THE00470
C ----- THE00480
C PI = 2.0 * DASIN(1.0D0) THE00490
C ANG = 1.00D-10 THE00500
C E = 1.6019D-19 THE00510
C MO = 9.1095D-31 THE00520
C H = 6.626D-34 THE00530
C HBAR = H/PI/2.0D0 THE00540
C K = 1.38066D-23 THE00550

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LIMIT = 10.00	THE00560
MC = 1.00	THE00570
NIV = 40	THE00580
	THE00590
C -----	THE00600
C READ IN THE RELEVANT PARAMETERS	THE00610
C -----	THE00620
	THE00630
	THE00640
C WRITE(6,10)	THE00650
C 10 FORMAT (3X,'PLEASE ENTER THE BARRIER WIDTH, HEIGHT AND WELL WIDTH	THE00660
C \$')	THE00670
C READ(5,*)BARW	THE00680
C READ(5,*)BARH	THE00690
C READ(5,*)WELW	THE00700
BARW=20.0000	THE00710
SUBARW=20.0000	THE00720
BARH=0.50000	THE00730
SUBARH=0.50000	THE00740
NWELLS=1	THE00750
C -----	THE00760
C DEFINE/GENERATE THE SUPERLATTICE WELL WIDTHS	THE00770
C -----	THE00780
C DO 12 I=1,NWELLS	THE00790
C SWIDTH(3)=84.90D-10	THE00800
C SWIDTH(2)=50.96D-10	THE00810
C SWIDTH(1)=36.79D-10	THE00820
C SWIDTH(1)=50.00D-10	THE00830
12 CONTINUE	THE00840
	THE00850
	THE00860
C WRITE(6,15)	THE00870
C 15 FORMAT (3X,'ENTER THE BARRIER AND WELL EFFECTIVE MASSES...')	THE00880
C READ(5,*)BEFM	THE00890
C READ(5,*)WEFM	THE00900
BEFM=0.1087D0	THE00910
WEFM=0.0670D0	THE00920
ND = 2.0D17	THE00930
TEMP = 300.000	THE00940
KTT = K * TEMP	THE00950
	THE00960
C -----	THE00970
C CALCULATE THE DENSITY OF STATES. THEN COMPUTE THE FERMI LEVEL	THE00980
C USING THE AYMERICH-HUMET APPROXIMATION TO F1/2. EC=0.	THE00990
C -----	THE01000
NC = 2.00*MC * ((2.00*PI*WEFM*MO*KTT/H/H)**1.5)/1.06	THE01010
	THE01020
EF = -31.469D-3 * E	THE01030
	THE01040
	THE01050
C -----	THE01060
C CONVERT UNITS TO M.K.S. SYSTEM	THE01070
C -----	THE01080
	THE01090
BEFM = BEFM * MO	THE01100

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WEFM = WEFM * MO	THE01110
	THE01120
BARW = BARW * ANG	THE01130
SUBARW = SUBARW * ANG	THE01140
	THE01150
BARH = BARH * E	THE01160
SUBARH = SUBARH * E	THE01170
	THE01180
C -----	THE01190
C LOOP THE APPLIED BIAS TO GET NIV 1-V POINTS.	THE01200
C -----	THE01210
DO 300 IV=1,NIV	THE01220
BIAS = 0.05000 + (IV-1)*0.00500	THE01230
C BIAS = 0.400000	THE01240
BIAS = BIAS * E	THE01250
	THE01260
C -----	THE01270
C SET UP ITERATION PARAMETERS FOR LOOPS	THE01280
C -----	THE01290
DE = BARH/350.DO	THE01300
	THE01310
THICK = 0.000000000000	THE01320
DO 40 I=1,NWELLS	THE01330
THICK = THICK + SWWDTH(I)	THE01340
40 CONTINUE	THE01350
	THE01360
THICK = THICK + 2.DO*BARW + DFLOAT(NWELLS-1)*SUBARW	THE01370
SLOPE = -BIAS/THICK	THE01380
ZETA = HBAR/SLOPE/2.000	THE01390
EE = 1.DO/3.DO	THE01400
CAMMA1 = -(-HBAR/BEFM*ZETA)**EE	THE01410
CAMMA2 = -(-HBAR/WEFM*ZETA)**EE	THE01420
CAMMA3 = CAMMA1	THE01430
ALFA1 = WEFM*CAMMA2/BEFM/CAMMA1	THE01440
ALFA2 = 1.DO/ALFA1	THE01450
	THE01460
RMASS = 2.DO*WEFM/HBAR	THE01470
BARG1 = BARW/CAMMA1	THE01480
	THE01490
BARG2 = BARW/CAMMA2	THE01500
	THE01510
	THE01520
C -----	THE01530
C SCANNING THE ELECTRON ENERGY	THE01540
C -----	THE01550
I = 0	THE01560
ENRGV = 0.00000 * E	THE01570
	THE01580
	THE01590
50 I = I + 1	THE01600
	THE01610
C DO 99 I=1.350	THE01620
	THE01630
	THE01640
ENRGV = ENRGV + DE	THE01650

BETA1 = (BARH-ENRGV)/CAMMA1/SLOPE	THE01660
BETA2 = (-ENRGV)/CAMMA2/SLOPE	THE01670
BETA3 = (SUBARH-ENRGV)/CAMMA1/SLOPE	THE01680
PHI11 = BETA1	THE01690
PHI12 = BETA1+BARG1	THE01700
	THE01710
	THE01720
PHI31 = (THICK-BARW)/CAMMA1 + BETA1	THE01730
PHI32 = THICK/CAMMA1 + BETA1	THE01740
	THE01750
KI = DSORT(ENRGV*RMAS/MBAR)	THE01760
KT = KI*DSORT(1.000 + BIAS/ENRGV)	THE01770
ALFA3 = WEFM/BEFM/CAMMA3/KT	THE01780
ALFA0 = KI*BEFM/CAMMA1/WEFM	THE01790
	THE01800
B11 = BID(PHI32)	THE01810
B12 = -BI(PHI32)/ALFA3	THE01820
B21 = -AID(PHI32)	THE01830
B22 = AI(PHI32)/ALFA3	THE01840
	THE01850
A11 = AI(PHI31)	THE01860
A12 = BI(PHI31)	THE01870
A21 = AID(PHI31)	THE01880
A22 = BID(PHI31)	THE01890
CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)	THE01900
	THE01910
	THE01920
X = (THICK-BARW)	THE01930
	THE01940
DO 75 IK=NWELLS,1,-1	THE01950
PHI = X/CAMMA2 + BETA2	THE01960
	THE01970
A11 = BID(PHI)	THE01980
A12 = -BI(PHI)/ALFA2	THE01990
A21 = -AID(PHI)	THE02000
A22 = AI(PHI)/ALFA2	THE02010
	THE02020
CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)	THE02030
	THE02040
X = X - SWDTH(IK)	THE02050
PHI = X/CAMMA2 + BETA2	THE02060
	THE02070
A11 = AI(PHI)	THE02080
A12 = BI(PHI)	THE02090
A21 = AID(PHI)	THE02100
A22 = BID(PHI)	THE02110
	THE02120
CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)	THE02130
	THE02140
IF (IK.EQ.1) GOTO 80	THE02150
	THE02160
PHI = X/CAMMA1 + BETA3	THE02170
	THE02180
A11 = BID(PHI)	THE02190
A12 = -BI(PHI)/ALFA1	THE02200

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      A21 = -A1D(PHI)
      A22 = A1(PHI)/ALFA1
      CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)
      X = X - SUBARW
      PHI = X/CAMMA1 + BETA3
      A11 = A1(PHI)
      A12 = B1(PHI)
      A21 = A1D(PHI)
      A22 = B1D(PHI)
      CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)
75      CONTINUE
80      A11 = B1D(PHI12)
      A12 = -B1(PHI12)/ALFA1
      A21 = -A1D(PHI12)
      A22 = A1(PHI12)/ALFA1
      CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)
      A11 = A1(PHI11)
      A12 = B1(PHI11)
      A21 = A1D(PHI11)
      A22 = B1D(PHI11)
      CALL MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)
      S = 2.DO*ALFA0/DCMPLX(ALFA0*B11+B22,ALFA0*B12-B21)
      S = S/(PI**(2*NWELLS+1))
      T = S * DCONJG(S)
      T = T*KT/KI
      R = 1.0D0/2.DO/ALFA0*S*DCMPLX(ALFA0*B11-B22,ALFA0*B12+B21)
      R = R * PI**(2*NWELLS+1)
      RAU = R * DCONJG(R)
      SUM = T + RAU
C .....
C *   DEFINE THE ARRAYS   *
C .....
C      TRANS(I)=T
      TRANS(I)=DLOG(T)
      REFLEC(I)=RAU
      ENERGY(I)=ENRGV
C      WRITE(6,97)ENRGV/E,T,RAU,SUM
C 97      FORMAT(2X,D12.5,4X,3D17.9)
C 100     CONTINUE
C -----

```

THE02210
 THE02220
 THE02230
 THE02240
 THE02250
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 THE02740
 THE02750

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```

C      CHECK FOR NEED TO CHANGE ENERGY INCREMENT.
C      -----
      IF (I.EQ.1) GOTO 50
      DELT = DABS( (TRANS(I)-TRANS(I-1))/TRANS(I-1)*100.DO )
      IF (DELT.GE.LIMIT.AND.T.GE.0.0001D-2)  DE=0.0001D0*E
      IF (DELT.LT.LIMIT.AND.T.LT.0.0001D-2)  DE=0.001*E
C      IF (ENRGV.GE.0.75D0*BARH) DE=0.001D*E
C      IF (ENRGV.GE.1.00D0*E)  GOTO 125
C      IF (ENRGV.GE.BARH)  GOTO 125
      GOTO 50
99  CONTINUE
125 CONTINUE
      NPNTS = 1
C      NPNTS = 350

      DO 150 I=1,NPNTS
C      DO 150 I=1,350
      WRITE(79,*)ENERGV(I)/E,TRANS(I)
      WRITE(80,*)ENERGV(I)/E,REFLEC(I)
150 CONTINUE

C      -----
C      FINISHED COMPUTING T FOR THIS BIAS. NOW GET CORRESPONDING CURRENT.
C      -----
      PREFIX = WEFM*E*KTT / 2.DO / PI/PI / HBAR/HBAR/HBAR
      SIGMA = TRANS(1)*D(ENERGV(1),EF,KTT,BIAS)*ENERGV(1)/1.0D0
      DO 200 IL=1,NPNTS-1
      TRAP = ( TRANS(IL)*D(ENERGV(IL),EF,KTT,BIAS) + TRANS(IL+1)*D(ENERGV(IL+1),EF,KTT,BIAS) ) * (ENERGV(IL+1)-ENERGV(IL)) / 2.DO
      SIGMA = SIGMA + TRAP
200  CONTINUE

      CURNT = PREFIX * SIGMA / 1.0D4

      JC(IV) = SNGL(CURNT)
      VOLT(IV) = SNGL(BIAS/E)

300 CONTINUE

C      -----
C      WRITE CURRENT DENSITIES IN DISSPLA FILES.
C      -----
      DO 400 I=1,NIV
      WRITE(81,*)VOLT(I),JC(I)
400 CONTINUE

      STOP
      END

C      -----
C      2X2 COMPLEX MULTIPLICATION SUBROUTINE
C      -----

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FILE: THESIS FORTRAN A BELL-NORTHERN RESEARCH

SUBROUTINE MAMULT(A11,A12,A21,A22,B11,B12,B21,B22)	THE03310
C11 = A11*B11 + A12*B21	THE03320
C12 = A11*B12 + A12*B22	THE03330
B21 = A21*B11 + A22*B21	THE03340
B22 = A21*B12 + A22*B22	THE03350
B11 = C11	THE03360
B12 = C12	THE03370
RETURN	THE03380
END	THE03390
C -----	THE03400
C DEFINE THE SUPPLY FUNCTION D(E,MU,KT,V)	THE03410
C -----	THE03420
DOUBLE PRECISION FUNCTION D(E,MU,KT,V)	THE03430
REAL*8 E,MU,KT,V,A	THE03440
A = 1.000 + DEXP((MU-E)/KT)	THE03450
A = A / (1.000 + DEXP((MU-E-V)/KT))	THE03460
D = DLOG(A)	THE03470
RETURN	THE03480
END	THE03490
	THE03500

C	-----	THE00010
C		THE00020
C	CALCULATES THE FERMI LEVEL WITH THE AID OF THE AYMERICH-MUMET	THE00030
C	ANALYTICAL APPROXIMATION TO THE FERMI INTEGRAL OF ORDER 1/2.	THE00040
C		THE00050
C	ASSUMES THAT SI IS THE DONOR IMPURITY AND ITS ACTIVATION ENERGY	THE00060
C	IS 0.0058 EV BELOW EC. GAAS BANDGAP IS FIXED WITH TEMP.	THE00070
C	-----	THE00080
C		THE00090
C	* DOUBLE PRECISION *	THE00100
		THE00110
	IMPLICIT DOUBLE PRECISION (A-H,L-Z)	THE00120
	REAL*8 MO,KI,KT,K,KTT,ZZ(800)	THE00130
	COMMON NC,PI,KTT,ED,ND	THE00140
C	-----	THE00150
C		THE00160
C	DEFINITIONS	THE00170
C	-----	THE00180
C	ED = DONOR IMPURITY LEVEL BELOW EC IN ELECTRON VOLTS.	THE00190
C	H = PLANCK'S CONSTANT	THE00200
C	HBAR = REDUCED VALUE OF PLANCK'S CONSTANT	THE00210
C	MO = FREE ELECTRON MASS	THE00220
C	MU = FERMI ENERGY WITH EC AS ZERO ENERGY REFERENCE.	THE00230
C	E = ELECTRON CHARGE	THE00240
C	TEMP = TEMPERATURE IN DEGREES KELVIN.	THE00250
		THE00260
		THE00270
C	-----	THE00280
C	CONSTANT VALUES	THE00290
C	-----	THE00300
	PI = 2.0 * DASIN(1.000)	THE00310
	ANG = 1.000-10	THE00320
	E = 1.60190-19	THE00330
	MO = 9.10950-31	THE00340
	H = 6.6260-34	THE00350
	HBAR = H/PI/2.000	THE00360
	K = 1.380660-23	THE00370
	LIMIT = 10.00	THE00380
	MC = 1.00	THE00390
	WEFM = 0.067000	THE00400
		THE00410
		THE00420
	ED = 0.0058 * E	THE00430
	ND = 1.0018	THE00440
		THE00450
C	DO 222 IT=50,400,10	THE00460
C	TEMP= IT	THE00470
		THE00480
	TEMP = 300.000	THE00490
	KTT = K * TEMP	THE00500
		THE00510
		THE00520
	ZZ(IT) = KTT * DLOG(DEXP(1.00/TEMP) - 1.00) / E * 1000.00	THE00530
		THE00540
		THE00550

FILE: THESIS2 FORTRAN A BELL-NORTHERN RESEARCH

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C ----- THE00560
C   CALCULATE THE DENSITY OF STATES. THEN COMPUTE THE FERMI LEVEL THE00570
C   USING NILLSON'S FULL RANGE APPROXIMATION TO ETA. EC=0. THE00580
C ----- THE00590
C   NC = 2.00*MC * ((2.00*PI*WEFM*MO*KTT/H/H)**1.5)/1.06 THE00600
C * THE00610
C * SUBROUTINE SOLVIT THE00620
C * IMPLICIT DOUBLE PRECISION(A-H,O-Z) THE00630
C * BETA=MAXIMUM/MINIMUM VALUE TO SOLVE FOR... THE00640
C * THE00650
C   ITRUE=0 THE00660
C THE00670
C   BETAMX= 0.400 * E / KTT THE00680
C   BETAMX= 1.00 THE00690
C   BETAMN=-0.6000 * E / KTT THE00700
C   BETAMN=-1.00 THE00710
C THE00720
C   DO 1000 I=1,10 THE00730
C THE00740
C     WRITE(5,*) I, ' BEST = ',BEST*KTT/E*1000.00 THE00750
C THE00760
C     IFIND=0 THE00770
C     BLAST= BETAMX THE00780
C     VALAST=FN( BETAMX ) THE00790
C     BSTEP= ( BETAMX-BETAMN )/100.000 THE00800
C THE00810
C     WRITE(5,*) ' BLAST ',BLAST THE00820
C     WRITE(5,*) ' VALAST ',VALAST THE00830
C     WRITE(5,*) ' BSTEP ',BSTEP THE00840
C THE00850
C     DO 1001 J=1,100 THE00860
C THE00870
C       B=BETAMX-DFLOAT(J)*BSTEP THE00880
C       VAL=FN(B) THE00890
C       WRITE(5,*) J, 'VAL= ',VAL THE00900
C       IF ((VAL*VALAST).LT.0.000) THEN THE00910
C THE00920
C         WRITE(5,*) 'J=',J THE00930
C         WRITE(5,*) 'ZERO CROSSING..... J=',J THE00940
C         IFIND=1 THE00950
C         BETAMX=B+BSTEP THE00960
C         BETAMN=B THE00970
C         RATIO=DABS(VALAST-VAL)/VALAST THE00980
C         IF (RATIO.GT.1.00-12) THEN THE00990
C           BEST=(VALAST/(VALAST-VAL))*(B-BLAST)+BLAST THE01000
C         ELSE THE01010
C           ITRUE=1 THE01020
C         ENDIF THE01030
C       ENDIF THE01040
C       IF (IFIND.EQ.1) GOTO 999 THE01050
C       VALAST=VAL THE01060
C THE01070
C 1001 CONTINUE THE01080
C THE01090
C 999 IF (ITRUE.EQ.1) GOTO 1002 THE01100
C 1000 CONTINUE

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FILE: THESIS2 FORTRAN A BELL-NORTHERN RESEARCH

C		THE01110
C1002	RETURN	THE01120
C1002	STOP	THE01130
1002	CONTINUE	THE01140
		THE01150
C	WRITE(81,*)TEMP,BEST/E*KTT*1000.DO	THE01160
	WRITE(5,*)TEMP,NC*FI(BEST)	THE01170
C	WRITE(80,*)TEMP,ZZ(IT)	THE01180
222	CONTINUE	THE01190
		THE01200
	STOP	THE01210
	END	THE01220
		THE01230
		THE01240
C	-----	THE01250
C	FERMI INTEGRAL OF ORDER 1/2.	THE01260
C	-----	THE01270
	DOUBLE PRECISION FUNCTION FI(N)	THE01280
	IMPLICIT DOUBLE PRECISION (A-M,K-Z)	THE01290
	COMMON NC,PI,KTT,ED,ND	THE01300
		THE01310
	XI = N + 2.13D0 + ((DABS(N-2.13D0))**2.4 + 9.6D0)**(5.D0/12.D0)	THE01320
	XI = 3.D0 * DSQRT(PI/2.D0) * XI**(-1.5)	THE01330
		THE01340
	FI = 1.D0 / (XI + DEXP(-N))	THE01350
C	WRITE(5,*) ' FI= ',FI*10.0D17	THE01360
		THE01370
	RETURN	THE01380
	END	THE01390
		THE01400
		THE01410
C	-----	THE01420
C	FUNCTION TO BE ZERO'ED.	THE01430
C	-----	THE01440
	DOUBLE PRECISION FUNCTION FN(N)	THE01450
	IMPLICIT DOUBLE PRECISION (A-M,K-Z)	THE01460
	EXTERNAL FI	THE01470
	COMMON NC,PI,KTT,ED,ND	THE01480
		THE01490
	FN = NC*FI(N) - ND/(1.D0 + 2.0D0*DEXP(N*ED/KTT))	THE01500
C	FN = NC*FI(N)	THE01510
C	WRITE(5,*) ' FN= ',FN	THE01520
		THE01530
	RETURN	THE01540
	END	THE01550

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