CHAPTER 1

THEORETICAL REVIEW

Tunneling of a particle through a barrier is one of the most studied phenomena in quantum mechanics. It plays an important role in many semiconductor devices. In particular, the tunnel diode or Esaki diode (Esaki 1958) involves tunneling through a forward-biased heavily doped (degenerate) junction in germanium. One important characteristics of the Esaki diode is that it exhibits negative differential resistance (NDR), making possible its application as a high frequency (microwave) oscillator. The properties of the original Esaki diode were determined (and hence also limited) mainly by the band structure of the bulk semiconductor. In 1973 Tsu and Esaki (Tsu and Esaki 1973) suggested that NDR can also be achieved in a superlattice. However, it took more than ten years before high quality quantum well (QW) samples exhibiting NDR could be fabricated (Sollner, Goodhue et al. 1983). Even in that case the sample involved a QW rather than a superlattice. NDR in GaAs/AlAs superlattice was reported several years later(Sibille, Palmier et al. 1990). Since this pioneering work NDR has been observed in many structures involving QWs and superlattices.

1.1. Peak – to – Valley Current Ratio (PVR)

PVR defined as the ratio of the current at the resonant tunneling peak energy to that at the minimum (or valley) before the current starts to increase again with voltage. The magnitude of this ratio is determined by scattering of the tunneling electrons within the well by phonons, interface roughness and other defects.

While the absolute peak-current densities resulting from simulations are in good agreement with experimental data, the calculated valley current densities are in one of more orders of magnitude lower than the experimental ones (Mizuta and Tanoue 1995). For AlAs/GaAs or AlAs/InGaAs diode structures on GaAs the experimental PVRs at room temperature are in the order of 6 (Waser 2005). The predicted PVR from simulations are more than one order of magnitude higher (Förster 2000). The reason for this discrepancy is the neglect of scattering effects in the calculation. Scattering effects broaden the resonance in the transmission probability while simultaneously damping it. The peak current density is nearly not sensitive to scattering effects but the valley current and the PVR are very strong influenced.

An appropriate scattering model is based on the Breit-Wigner generalization of the Lorentzian form of the resonant transmission probability. Within this formalism resonant tunneling in one dimension is studied by Stone *et al.*(Stone and Lee 1985) who derived the total transmission probability in the presence of inelastic scattering for a symmetric structure as:

$$T_{tot} = \frac{\frac{1}{4}\Gamma_0\Gamma}{\left(E - E'\right)^2 + \frac{1}{4}\Gamma^2} \qquad (0.1)$$

Where Γ_0 is the half width of the resonance in the coherent transmission probability and $\Gamma = \Gamma_0 + \Gamma_i$ is the total resonant half width, Γ_i representing the contribution to the broadening due to the inelastic scattering. Büttiker (Buttiker 1988) has interpreted this total transmission probability as a sum of a coherent and sequential (incoherent) transmission probabilities

$$T_{tot} = T_c + T_i \qquad (0.2)$$

In this picture of scattering the fraction of carriers penetrating the structure coherently is $T_c/T_{tot} = \Gamma_0/\Gamma$ and the fraction of carriers traversing the structure sequentially is

$T_i/T_{tot} = \Gamma_i/\Gamma$. From these results one can infer that the smaller the elastic width Γ_0, the smaller is the amount of scattering needed to make the sequential tunneling current dominant. This means that in tunneling diode with thick barrier (sharp resonances) in spite of small scattering probability, considerable sequential tunneling contributions will be observed. Furthermore, Eq.(0.1) can be interpreted as a folding of the coherent transmission probability (Eq.(0.1) with $\Gamma_i = 0$) with a normalized Lorentzian of half width Γ_i. In current density calculations this mechanism conserves the peak current density but affects the valley current very strongly resulting in lower PVR values. In this kind of treatment of I-V curves the effect of scattering is used as a fitting parameter to determine the resonance broadening at room temperature. For a typical RTD with 6 ML AlAs barriers and a 5 nm GaAs quantum well a resonance half width of about 8 meV at room temperature was found(Waser 2005).

From the theoretical point of view this treatment of scattering is not satisfactory. Therefore a more complex approach is needed. In an enhanced calculation non-equilibrium Green-function theory is the base of the calculations in which self-consistent charging, incoherent and inelastic scattering, and the band structure is considered. Lake *et al.*(Foster 1994) have developed a complex simulation package in which most of the relevant effects are taken into account. A real-space tight binding formulation provides an accurate synthesis of heterostructures on an atomic scale. It implies the consideration of inter-valley and inter-band transitions and gives a sophisticated description of electrons in the gap-region ("band-warping").

The calculations of Peak to Valley Ratio (PVR) showed a good agreement with the experimental results at the peak (Tsuchiya and Sakaki 1986). In the contrary, the calculated valley current density is far smaller than that is observed in the experiment, and thus the resulting P/V current is more than one order of magnitude larger than the experimental data. The excess current observed in the valley regime has been ascribed to phase-coherence breaking scattering, which is neglected in the global coherent tunneling model.

A sequential tunneling model was proposed by Luryi (Luryi 1985; Luryi 1989), based on the idea that the mean free time of electrons in a bulk GaAs material is of the order of subpicoseconds at room temperature, which can be much shorter than the dwell time of relatively thick double-barrier structure. For instance, the momentum relaxation time of electrons in a low-doped n-type GaAs bulk material ($N_D = 10^{14}\ cm^{-3}$) is of the order of 0.1 ps for a wide range of energy (Mizuta and Tanoue 1995). So it is likely that the electrons in quantum well experience some degree of scattering during tunneling process and lose their phase-coherence. This alternative explanation of the RTD phenomenon came out about ten years after the global coherent resonant tunneling reported by Tsu and Esaki.

1.2. $\mathbf{T_0}$ Effect and Inhomogeneous Barrier Height

The current diffusion ideality can be studied by the ideality factor n. The closer the ideality factor to unity the more ideal the diffusion is. Ideality factor can be found by plotting $\ln J$ against V and taking the slope of the plot as;

$$n \equiv \frac{q}{kT} \frac{\partial V}{\partial(\ln J)} \tag{0.3}$$

Where J is the current density, q is the charge unit, k is Boltzmann constant in eV/K, and T is temperature in kelvin. Often it has been found that the ideality factor increases with decreasing temperature.

T_0 effect is a way to study the dependency of the ideality factor on the temperature. Such a dependence could be attributed to the inhomogenities in the barrier height(Pipinis, Rimeika et al. 1998). And the existence of the thermionic field emission current.

Apparent barrier height or zero bias barrier height can be found from equation (1.8) which depends on the saturation current.

According to Tung's theory, there is a linear correlation between the experimental zero bias barrier heights ϕ_{B0} and ideality factor n.

Altuntas et al. (Altuntas, AltIndal et al. 2009) experimental results show that there are two linear regions between ϕ_{B0} and n which they explained as a literal inhomogeneities of the barrier height.

On the other hand, Rodrigues(Rodrigues 2007) has a linear relation but the ideality factor was larger than 4. This problem has been explained as surface states in the Chemical vapor deposition (CVD) contacts which tend to be inhomogeneous.

The barrier height obtained under flat-band condition is called the flat-band barrier height and is considered as the real essential quantity. The flat band barrier height ϕ_{bf} can be calculated from the experimental ideality factor and zero-bias barrier height ϕ_{b0} according to(Werner and Guttler 1993)

$$\phi_{bf} = n\,\phi_{b0} - (n-1)\frac{kT}{q}\left(\frac{N_C}{N_D}\right) \qquad (0.4)$$

Where N_C is the density of states in the conduction band and N_D is the doping concentration in the semiconductor.

Usually, the barrier height obtained under the flat band condition is considered to be a real quantity which assumes that the electrical field is zero. This eliminates the effect of image force lowering that would affect the I-V characteristics and removes the influence of lateral in homogeneity(Dökme, Altindal et al. 2006). To address the observed abnormal deviation from classical thermionic emission theory, some researchers (Schmitsdorf, Kampen et al. 1995; AltIndal, Karadeniz et al. 2003) considered a system of discrete regions of low barrier imbedded in a higher background uniform barrier.

Barrier In homogeneities are described mainly by Gaussian distribution function (Karatas and AltIndal 2005)

$$P(\phi_b) = \frac{1}{\sigma_S \sqrt{2\pi}} \exp\left(-\frac{\left(\phi_b - \bar{\phi}_b\right)^2}{2\sigma_S^2} \right) \qquad (0.5)$$

Where σ_S is the standard deviation, ϕ_b is the barrier height and $\bar{\phi}_b$ is the mean barrier height.

The total current across the Schottky diode containing barrier inhomogeneities can be expressed as (Karatas and AltIndal 2005)

$$I(V) = \int_{-\infty}^{+\infty} I(\phi_b, V) P(\phi_b)\, d\phi \qquad (0.6)$$

Where $I(\phi_b, V)$ is the current at voltage bias V for a barrier of height ϕ_b and $P(\phi_b)$ is the normalized distribution function giving the probability of occurrence for barrier height ϕ_b.

Using Eq. (0.6), the total current in a given forward bias V is then given by (Karatas and AltIndal 2005)

$$I(V) = A^{**}T^2 \exp\left[-\frac{q}{kT}\left(\bar{\phi} - \frac{q\sigma_S^2}{2kT} \right) \right] \exp\left(\frac{qV}{n_{ap} kT} \right) \left[1 - \exp\left(-\frac{qV}{kT} \right) \right] \qquad (0.7)$$

With

$$I_0 = AA^{**}T^2 \exp\left(-\frac{q\phi_{ap}}{kT}\right) \tag{0.8}$$

Where n_{ap} and ϕ_{ap} are the apparent ideality factor and apparent barrier height, respectively, and are given by

$$\phi_{ap} = \bar{\phi}_{ap}\left(T = 0\right) - \frac{q\sigma_{so}^2}{2kT} \tag{0.9}$$

$$\left(\frac{1}{n_{ap}} - 1\right) = \rho_2 - \frac{q\rho_3}{2kT} \tag{0.10}$$

We need to assume the mean Schottky barrier $\bar{\phi}_b$ and σ_s are linearly bias-dependent on Gaussian parameters, such that $\bar{\phi}_b = \bar{\phi}_{b0} + \rho_2 V$ and standard deviation $\sigma_s = \sigma_{so} + \rho_3 V$, where $\bar{\phi}_{b0}$ is the barrier height at temperature $T = 0\ K$, ρ_2 and ρ_3 are voltage coefficients which may depend on temperature, quantifying the voltage deformation of the barrier height distribution (Zhu, Detavernier et al. 2000; Gumus, Turut et al. 2002). The temperature dependence of σ_s is small and therefore can be neglected (Hudait, Venkateswarlu et al. 2001). The decrease of zero-bias barrier height is caused by the existence of the Gaussian distribution and the extent of influence is determined by the standard deviation itself. The existence of the barrier inhomogeneities affects the current transport of electrons across the Schottky barrier. Since at low temperatures, charge carriers have very low energies to surpass the energy barrier, tunneling of electrons is the dominant process(Mtangi, Auret et al. 2009).

As a result of the Gaussian distribution of the barrier, Richardson plot can now be modified by combining Eqs. (0.8) and (0.9) such that,

$$I_s = AA^{**}T^2 \exp\left[-\frac{q\bar{\phi}_{ap}}{kT} + \frac{q^2\sigma_{so}^2}{2k^2T^2}\right] \qquad (0.11)$$

And

$$\ln\left(\frac{I_0}{T^2}\right) - \left(\frac{q^2\sigma_{so}^2}{2k^2T^2}\right) = \ln\left(AA^{**}\right) - \frac{q\phi_{ap}}{kT} \qquad (0.12)$$

Where A^{**} is the modified Richardson constant. A plot of the modified $\ln(I_0/T^2) - (q^2\sigma_{so}^2/2k^2T^2)$ versus $1000/T$ yields a straight line with the slope giving the mean barrier height and the intercept giving the modified Richardson constant.