QUANTUM FUNCTIONALITY OF NANOELECTRONICS DEVICE STRUCTURES
(Funcionalidad Cuántica en la Estructura de los Dispositivos Nanoelectrónicos)

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ABSTRACT: Physical limits of the present day microelectronics are discussed and arguments given, why working principles of conventional transistor-based designs will fail. Theoretical concepts are applied to quantum functional devices and their requirements for basic properties, like quantization and coupling effects, carrier transport as well as time constants.

RESUMEN: Se discuten los límites físicos de la microelectrónica actual, y se presentan razones del porque los principios de operación de transistores convencionales en el futuro fallarán. Se aplica conceptos teóricos para dispositivos funcionales cuánticos y sus condiciones para propiedades básicas, como efectos de cuantización y de acoplamiento, transporte de portadores de carga y constantes de tiempo.

Keys Words: nanoelectronic, quantum functionality, Tunneling of electrons

I. INTRODUCTION

Quantum-size effects in semiconductors and their applications in digital functional devices are decisive aspects of the concept for a future generation of integrated circuits, approaching ultimate physical limits [Chang, 200], [Hiramoto, 2000].

From today's point of view there are still a lot of questions concerning the theory and fabrication of complex functional quantum devices and circuit. [Zehe, 2000], [Sze, 1997]

Interdisciplinary knowledge is essential to address these challenging problems. Device engineers and circuit designers link their work to related work in physics, and vice versa. Neither physicists nor device engineers and system experts can take present process technologies for granted. An independence of successive development steps as in the field of current conventional transistor-based technologies is hardly foreseeable at present. Fundamentals of physics, electronics and system architecture have to be assessed according to engineering aspects, such as scaling capability, functional density, power-delay time product, and thus maximum achievable chip complexity and functional throughput. [claro et al, 1997], [Hayashi et al, 1990]

The objective of the present paper consists in a discussion of physical fundamentals which dominate the microelectronics to nanoelectronics transition.

II. EXPONENTIAL TRENDS AND LIMITS OF TRANSISTOR BASED APPROACHES

Since the realization of the first integrated circuit in 1959 the number of devices per chip has been increased by about two orders of magnitude per decade by increasing packing efficiency and by enlarging the chip area.

These trends can be approximated by exponential functions. As an example, the feature size η may be given by:

$$\eta = 2\mu m \cdot e^{-0.135(t-1980)} \qquad (1a)$$

Ignoring scaling limits, one obtains, by extrapolation from eq. 1a minimum lateral dimensions of about 130 nm in 2000, respectively. Assuming no further increase in chip size and packing efficiency, but sustaining the 100-fold increase in chip complexity per decade, yield two even more progressive scaling laws.

$$\eta = 0.53\mu m \cdot e^{-0.23(t-1990)} \qquad (1b)$$
$$\eta = 0.53\mu m \cdot e^{-0.23(t-1985)} \qquad (1c)$$

Using eq. 1c, minimum geometries of 100 nm had been reached in the mid-'90s and 30 nm will be required at the beginning of the new century (see fig. 1).

The working principles of conventional transistors and architectures will begin to fail in this size regime because:

(i) carrier transport control using depletion layers created by electrostatic potentials is degraded, so that sub-threshold currents and punch-through will affect device behavior, and

(ii) quantum mechanical effects, like quantum tunneling come into play over distances comparable to, and smaller than the DeBroglie wavelength of conduction electrons. Electrons can tunnel through potencial barriers, devices, and isolation between devices starts to fail.
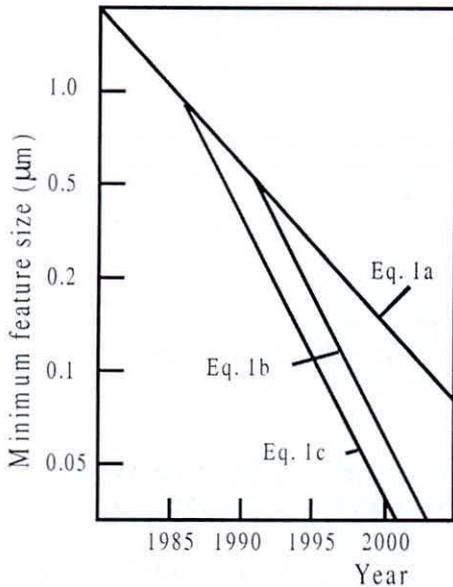

Fig. 1: Minimum feature size versus calendar year for different exponential fittings.

III. TUNNELING OF ELECTRONS THROUGH POTENTIAL BARRIERS

The transmission probability of electrons tunneling through a potential barrier is given by a transmission coefficient T depending on the shape of the barrier and the electron energy. For barriers with height V_{oz}, width b, and impacting electrons with energy E_z, a modified WKB-approximation formula (WKB: Wentzel - Kramers - Brillouin) for rectangular barriers gives the transmission coefficient T as the ratio between the amplitudes of the transmitted and the incident wave:

$$T(E_z) = \left\{ 1 + 0.25(k_{1z}/k_{2z} + k_{2z}/k_{1z})^2 \cdot \sinh^2(k_{2z}b) \right\}^{-1}$$

(2)

where:

$$k_{iz} = \sqrt{2m_n \cdot E_z}/\hbar, \quad k_{2c} = \sqrt{2m_n(V_{0z} - E_c)}/\hbar$$

(3)

Fig. 2 shows the transmission coefficient T in the region of, and below the DeBroglie wavelength $\lambda = h/\sqrt{2m_n \cdot E_z}$ of conduction electrons. Today most experts agree that minimum lateral dimensions will eventually saturate for high volume IC's in the 0.1 μm and 0.2-0.4 μm range for conventional devices and circuits, respectively. The limitations on circuit geometries are mainly due to isolation and interconnection problems.

These projections have triggered an intensive search for alternatives to conventional transistor-based microelectronics to sustain exponential trends in chip complexity over the next decades. Intensive investigations into physics, electronics, system architectures and processing requirements have been underway since the beginning of the '80s.
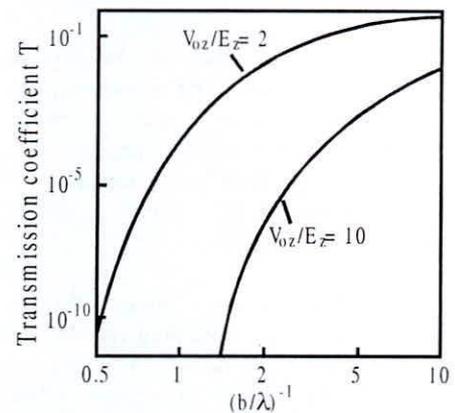

Fig. 2: Transmission coefficient versus wavelength of conducting electrons calculated by the WKB formula.

IV. BEYOND EVOLUTIONARY APPROACHES

The fundamental idea is to make use of precisely those quantum mechanical effects, as e.g. quantum tunneling, which cause the failure of conventional transistor-based technologies. This concept may lead eventually to complex functional devices based on quantum mechanical effects. The basic structure is the resonant tunneling double barrier. The term "nanoelectronics" was introduced in order to identify the realization of quantum devices in alternative architectures.

Quantum mechanical effects dominate nanoelectronics structures. The aim of this presentation is to apply well-known theories to the requirements of quantum functional devices and to provide qualitative conclusions on patterned geometries, carrier transport, lateral quantization effects, coupling effects and time constants of resonant tunneling structures, generally excluding scattering (coherent resonant tunneling). An exact analysis of complicated quantum transport processes in real structures requires extensive models, including knowledge of scattering mechanisms, self-consistent potentials, the distribution of electrons at the tunneling interfaces, real band structure, as well as an

extensive mathematical formalism, e.g. transfer- and scattering matrix techniques or methods for direct solutions of the Schrödinger or Wigner-function transport equations (see Tab. 1).

V. EFFECTIVE MASS APPROXIMATION

The effective mass approximation gives an analytical, so-called WKB formula which allows to determine transmission coefficients for potential barriers. This formula is simple, andshould be sufficient to obtain the desired qualitative results needed for the discussion in this paper. [Yuan & Seabaugh, 1999]

The material system considered here generally $GaAs / Al_xGa_{1-x}As$, where $m_n = (0.067 + 0.083x) \cdot m_o$ and $\Delta E_c = x \cdot 1eV$.

Table 1

Physical model	Methode	Feature
Effective mass Approximation	• Transfer matrix technique	• Applied to zero dimensional electron systems (quantum dots) • Subband mixing due to lateral wave-function mismatch • Multichannel transport [Kei ko, 1998]
	• Scattering matrix technique	• Stable for large finite multiple barrier systems • Effects of various conduction band minima and interband transference. [Maine, 1998]
	• Finite differences	• Applied to transient and small signal analysis. [Heilmeier, 1984]
	• Semiclassical perturbation theory	• Applied to small signal analysis. [Sokolovski, 1988]
	• Crank-Nicholson type methods	• Applied to transient analysis. [Guo et al, 1988]
Tight binding approximation	• Green's function technique	• Including scattering. [Kim et al, 1988]
	• Green's function and	• Including scattering. • Applied to disorder effects. [Schulz, 1988]
	transfer matrix technique	
Wigner function, Poisson's equation		• Including scattering • Including self-consistent potentials • Applied to transient analysis. [Kluksdahl, 1989]
Pseudopotential matrix		• Applied to momentum mixing and zone folding effects due to reduced dimensionality. [Jaros et al, 1987]

Fig. 3 shows the electron energy diagram of a basic resonant tunneling double barrier in thermal equilibrium (a). For a certain applied bias V, (b), electrons with three degrees of freedom (3-DOF) in the left degenerately doped emitter (emitter Fermi-sphere) can tunnel resonantly through the unoccupied levels of the two-dimensional sub band in the well (shaded disk). This basic structure is fabricated by one-dimensional patterning of solids.
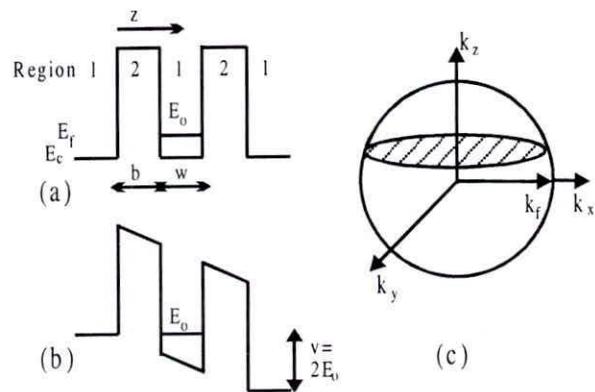

Fig. 3: Electron energy diagram in equilibrium (a) and in resonance (b) of a double barrier resonant tunneling diode. The sphere (c) illustrates the operation in momentum space.

Electron systems of reduced dimensionality are of great importance for future quantum functional devices, requiring two-dimensional (quantum wire) and three-dimensional (quantum dot) patterning of single-crystal solids.

The present and probably future supremacy of the heterostructure tunneling configuration is due to its outstanding ability to modulate the lattice potential abruptly within one or a few monolayers, and thus to create band discontinuities.

VI PATTERNED GEOMETRIES

Resonant tunneling effects, in order to be clearly observable, require both (i) and (ii):

(i) An energy gap between discrete states in the well, which is larger than the average thermal energy kT. Fig. 4 shows a transition region between kT and 4 kT using the energy gap between ground (E_o) and the first excited (E_1) state. The subband energy is given by the solution of the Schrödinger equation for finite barrier height:

$$-\frac{\hbar^2}{2} \cdot \frac{\partial}{\partial_z}\left[\frac{1}{m_n(z)} \cdot \frac{\partial \psi}{\partial_z}\right] + E_{pot}(z) \cdot \psi = E\psi, \quad (4)$$

where $E_{pot1} = V_{oz}$, $m_{n1} = 0.11m_o$, and $E_{pot2} = 0$, $m_{n2} = 0.067 m_o$.
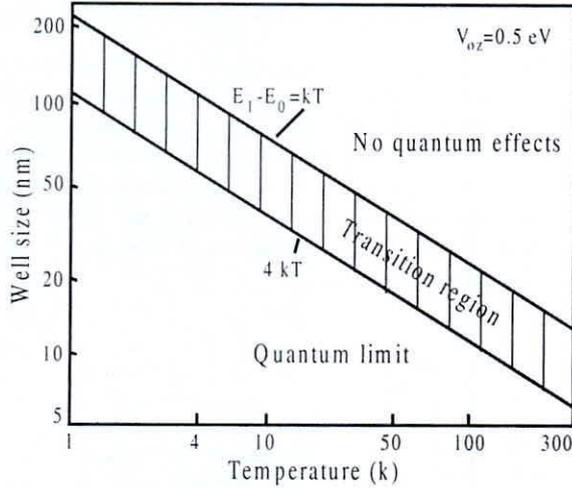
Fig. 4: Well size regimes for GaAs/AlGaAs quantum devices versus temperature.

The transition region is situated between 5.4 and 11.5 nm, and between 11.3 and 24 nm well width at room temperature or liquid nitrogen temperature, respectively. The 0.1 μm limit is not exceeded until liquid helium temperature is reached.

(ii) Sufficient transmittance of potential barriers given by the transmission coefficient T. The Wentzel-Kramers-Brillouin (WKB) approximation is valid, when the potential varies smoothly. It can however be adapted to abruptly varying potentials like rectangular barriers, in reasonable agreement with the transfer matrix technique, by adding a prefactor to the expression. The same factor is obtained by solving the Schrödinger equation (eq. 4) for rectangular barriers (eq. 2). Assuming $k_{2z}b \gg 1$ the transmission coefficient is then given by

$$T(E_z) = \frac{16 \cdot \exp(-2k_{2z}b)}{\left(k_{1z}/k_{2z} + k_{2z}/k_{1z}\right)^2}. \quad (5)$$

Fig. 5 shows right (T_r) and left (T_l) transmission coefficients of the double barrier structure in fig. 3(b) as a function of the subband energy E_o, assuming an average electron energy E_z

$= E_o/3$ and $E_z = 5/3E_o$ for the right and left hand side barriers, respectively. Both, barrier and well width are 5 nm.

The transmission coefficient T_o of the whole structure in resonance is

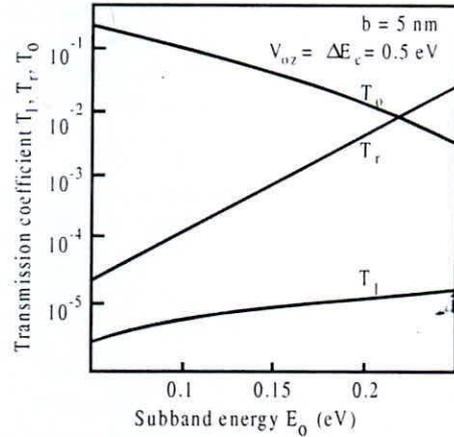$$T_o \cong 4T_r \cdot T_l /(T_r + T_l)^2 \quad (6)$$

Fig. 5: Transmission coefficient of left, right, and double barrier in resonance as a function of resonant energy E_o

while the lifetime width of the resonant state is given by:

$$\Delta E_o \cong E_o \cdot (T_r + T_l) \quad (7)$$

The calculations are based on coherent tunneling, although neglecting effects of electron scattering is only possible as far as the scattering time (relaxation time):

$$\bar{\tau} = \mu \cdot m_n / q \quad (8)$$

is much larger than the lifetime of a resonant state:

$$\tau_d = \hbar / \Delta E_o. \quad (9)$$

The condition $\tau_d = \bar{\tau}$ is indicated in Fig. 6 by the shaded region. For smaller barriers dominates coherent tunneling. Using typical low-field mobilities of a two-dimensional electron gas in selectively doped GaAs/AlGaAs heterojunctions gives maximum dimensions of rectangular potential barriers in the 1.5-5.5 nm range for coherent resonant tunneling at room temperature, and in the 3-9 nm range at 77 K.

Phase coherence is destroyed by both elastic scattering of carriers, inhomogeneities, alloying effects and inelastic scattering by phonons. Broadening of resonant states leads to broadening (and reduction) of the transmission peak

$$T(E_z) = \frac{\Delta E_o^2 \cdot T_o(E_z)}{(E_z - E_o)^2 + \Delta E_o^2} \qquad (10)$$
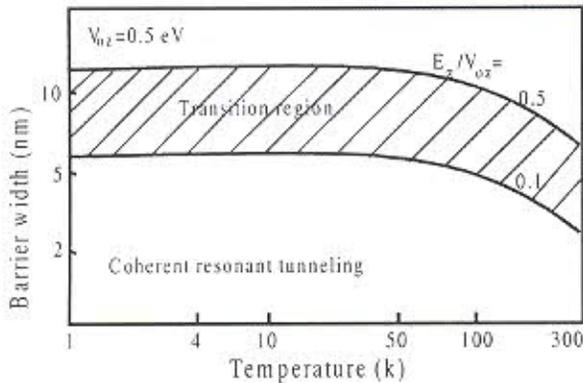

Fig. 6: Barrier size requirements for coherent resonant tunneling in $Al_xGa_{1-x}As/GaAs$ (x=0.5 double barrier structure

If inelastic phonon scattering totally destroys the wave coherence, a cancellation of net reflected waves will no longer be possible (Fabry-Perot resonator). Phase-randomizing interactions remove the correlation of transport processes between the right and left hand side barriers.
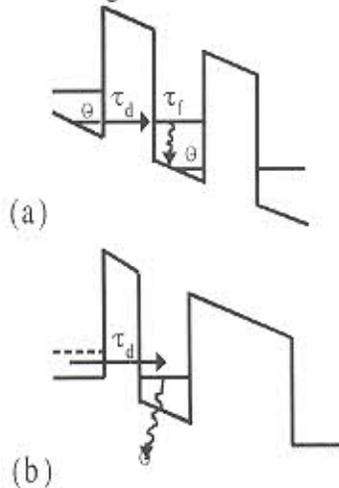

(a)

(b)

Fig. 7: Schematic diagram of different sequential resonant tunneling mechanisms

A sequential approach is more appropriate. From the viewpoint of device designer, a possible distinction between two resonant tunneling mechanism opens a new field for the discussion of such devices. Coherent tunneling is a property of the double barrier as a whole, and definitively requires two interacting tunneling steps.

Assuming sequential resonant tunneling, the device engineer is free to decide upon further processing of charge carriers after the first tunneling step, e.g. transport perpendicular to the former tunneling direction may be possible (see fig. 7).

VII. SUMMARY

A quantum mechanical approach to a new class of integrated circuits will dominate future device architecture and process technologies on an atom – by - atom implementation and control level.

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