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THERMIONIC EMISSION IN HETEROJUNCTIONS

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SUMMARY

The thermionic emission is one of the main conduction mechanisms in heterojunctions. In order to perform realistic numerical simulation of III-V devices a model of thermionic emission at the interface between two semiconductors is proposed. This model, derived from the thermionic emission-diffusion theory, is applied to some typical heterostructures such as those encountered in optoelectronic components.

INTRODUCTION

Many of today III-V components are heterostructures such as laser diodes, photodiodes, high electron mobility transistors, bipolar heterojunction transistors (Milnes 1986). Specific simulation problems are encountered when dealing with the description of heterojunctions. For instance Fermi-Dirac statistics description of free carriers must be used in most of the above devices owing to the notchs and spikes appearing at heterointerfaces (Viallet, Mottet 1985). Simulation of the conduction through heterojunction is an other problem which must be dealt with.

The well known drift-diffusion model, which is extensively used to describe the conduction in semiconductor devices, is scarcely adequate to take into account the effective conduction mode at the heterojunction. Among the possible conduction mechanisms, thermionic and tunnel emissions are the most often encountered mechanisms at heterojunctions

(Milnes, Feucht, 1972). A usable model of the thermionic emission has already been described to simulate the metal-semiconductor Schottky diode (Baccarani, 1986). Typically such a model allows to describe the behaviour of the MESFET Schottky diode gate.

In this paper we propose a model to simulate the thermionic emission at the interface between two semiconductors. This model is fully compatible with the drift-diffusion model that we already proposed to describe conduction in graded heterojunctions.

THEORETICAL APPROACH

The general set of equations used to describe steady state conduction in semiconductors is composed of Poisson equation and continuity equations:

$$\mathrm{div}(\epsilon\cdot\overrightarrow{\mathbf{grad}}\ \varphi) = q\cdot(n - p - C) \tag{1}$$

$$-\frac{1}{q}\cdot\mathrm{div}\ \overrightarrow{J_n} = G_e - U \tag{2}$$

$$\frac{1}{q}\cdot\mathrm{div}\ \overrightarrow{J_p} = G_e - U \tag{3}$$

Where C is the net fixed charge density. G_e is the electron-hole pair generation term due to external interaction such as light absorption. U is the recombination generation term due to deep centers, Auger or band to band capture emission processes. The currents in isothermal graded heterojunctions are described by the drift diffusion model:

$$\overrightarrow{J_n} = -q\cdot n\cdot\mu_n\cdot\overrightarrow{\mathbf{grad}}\ \varphi_n \tag{4}$$

$$\overrightarrow{J_p} = -q\cdot n\cdot\mu_p\cdot\overrightarrow{\mathbf{grad}}\ \varphi_p \tag{5}$$

Where φ_n and φ_p are the electron and hole electrochemical potentials used in the Fermi-Dirac distribution function. In most of the heterojunctions the Maxwell-Boltzmann statistics are unsuitable to describe carrier densities because of the spike and notch which exist at the interface. So the carrier densities are described by the Fermi-Dirac statistics in the parabolic band assumption:

(6) $$n(\varphi,\varphi_n) = N_C \cdot \mathcal{F}_{1/2}\left(\frac{q\cdot\varphi + \chi - q\cdot\varphi_n}{k\cdot T}\right)$$

(7) $$p(\varphi,\varphi_p) = N_V \cdot \mathcal{F}_{1/2}\left(\frac{-q\cdot\varphi - \chi - E_g + q\cdot\varphi_p}{k\cdot T}\right)$$

Where χ is the electron affinity and E_g the band gap energy of the local semiconductor. The $\mathcal{F}_{1/2}$ Fermi integral can be described with appropriate approximations. Viallet (1985) showed how this set of equations can be solved with respect to φ, φ_n, φ_p as main unknowns.

If abrupt heterojunction interfaces are considered, the possible conduction mechanisms are thermionic emission and tunnel effect. The tunnel emission occurs in heavily doped semiconductors which induce very high electric field regions at the interface. For low doped semiconductors, the thermionic emission governs the conduction in the room temperature range. A model of thermionic emission has already been described by Baccarani (1986) for the metal-semiconductor Schottky diodes. This model is derived from the thermionic emission-diffusion theory proposed by Crowell and Sze in 1966. This theory is used to describe the thermionic emission at the interface between two different semiconductors. Let us consider the electron conduction at the interface between semiconductor a and semiconductor b such as $\chi_a > \chi_b$. Figure 1a shows the bottom of the conduction band E_C and the electron Fermi level $-q\cdot\varphi_n$ at thermodynamic equilibrium. The electrons which can flow from a to b need to have enough energy to overcome the barrier height due to conduction band discontinuity. On the opposite electrons can directly flow from b to a and this current flow is:

$$J_{b\to a} = v_{nb} \cdot n_{b0}$$

where $n_{b0} = n_b(\varphi_b,\varphi_n)$ is the carrier density, v_{nb} the electron thermal velocity, φ_b and φ_n the electrostatic and electrochemical potentials in semiconductor b.

At thermodynamic equilibrium $J_n = -q\cdot(J_{a\to b} - J_{b\to a}) = 0$ so that the electon flow from a to b is $J_{a\to b} = J_{b\to a}$.

Under bias condition, as shown on figures 1b and 1c, the electron flow from b to a is

$$J_{b\to a} = v_{nb}\cdot n_b(\varphi_b, \varphi_{nb}).$$

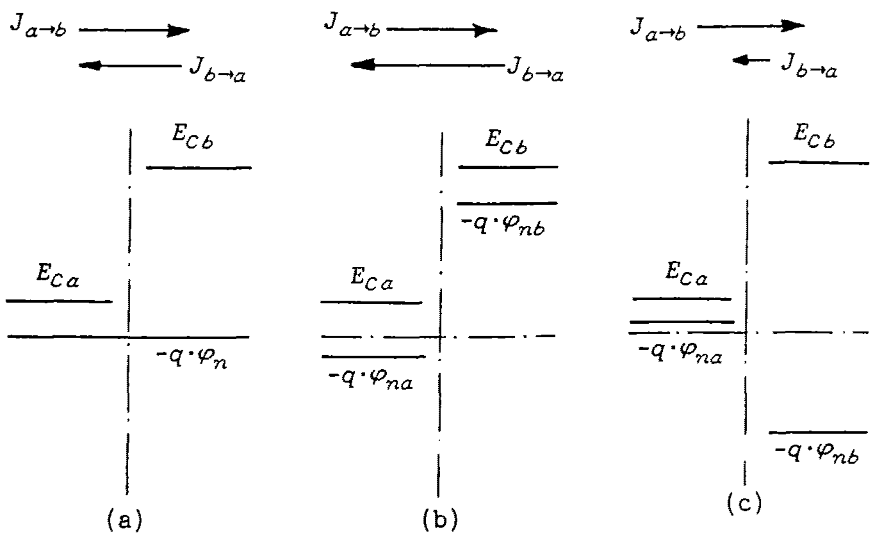

Fig. 1. Isotype heterojunction interfaces. a) Thermodynamical equilibrium. b) Forward bias. c) Reverse bias.

The electron Fermi level $-q\cdot\varphi_{na}$ on the a side has changed with regard to the thermodynamic equilibrium. This is the main difference with the metal-semiconductor case. To calculate the electron current $J_{a\to b}$, let us imagine the Fermi level $-q\cdot\varphi_{nb}$ equal to $-q\cdot\varphi_{na}$ on the b side of the interface. Therefore the whole current $J_n = 0$, which implies that the electron flow from a to b is equal to the flow of electrons from b to a calculated with $\varphi_{nb} = \varphi_{na}$

$$J_{a\to b} = v_{nb}\cdot n_{b0} \text{ with } n_{b0} = n_b(\varphi_b, \varphi_{na})$$

The electron current is then

(8) $$J_n = -q\cdot v_{nb}\cdot(n_b - n_{b0})$$

where

(9) $$n_b = N_{Cb} \cdot \mathcal{F}_{\frac{1}{2}}\left(\frac{q\cdot\varphi_b + \chi_b - q\cdot\varphi_{nb}}{k\cdot T}\right)$$

(10) $$n_{b0} = N_{Cb} \cdot \mathcal{F}_{\frac{1}{2}}\left(\frac{q\cdot\varphi_b + \chi_b - q\cdot\varphi_{na}}{k\cdot T}\right)$$

In fact on the b side of the interface, the Maxwell-Boltzmann statistics could be used instead of Fermi-Dirac since $E_{Cb} - q\cdot\varphi_{nb}$ is larger than $k\cdot T$. With that assumption

(11) $$n_{b0} = n_b \cdot exp\left(\frac{q\cdot\varphi_{nb} - q\cdot\varphi_{na}}{k\cdot T}\right)$$

and

(12) $$J_n = -q\cdot v_{nb}\cdot n_b \cdot \left[1 - exp\left(\frac{q\cdot\varphi_{nb} - q\cdot\varphi_{na}}{k\cdot T}\right)\right]$$

For large forward bias the condition $E_{Cb} - q\cdot\varphi_{nb}$ larger than $k\cdot T$ may not be verified. But in that case $n_b \gg n_{b0}$ so that the error on the current is totally negligeable but n_b must be expressed using (9).

For a Maxwellian distribution on the b side of the interface, the thermal velocity v_{nb} is given by (Crowell and Sze, 1966)

(13) $$v_n = \frac{\int_0^{\infty} v_x \cdot exp\left(\frac{- m_n^* \cdot v_x^2}{2\cdot k\cdot T}\right)\cdot dv_x}{\int_{-\infty}^{\infty} exp\left(\frac{- m_n^* \cdot v_x^2}{2\cdot k\cdot T}\right)\cdot dv_x} = \sqrt{\frac{k\cdot T}{2\cdot m_n^* \cdot \pi}} = \frac{A_n^* \cdot T^2}{q\cdot N_C}$$

where m_n^* is the effective mass and A_n^* the effective Richardson constant for electrons.

At heterojunctions both electron and hole thermionic emissions occur. The hole thermionic emission at the valence band discontinuity is established in a similar way to electron emission. If $\chi_a + E_{ga} < \chi_b + E_{gb}$ the hole current expression is

(14) $$J_p = q\cdot v_{pb}\cdot p_b \cdot \left[1 - exp\left(\frac{- q\cdot\varphi_{pb} + q\cdot\varphi_{pa}}{k\cdot T}\right)\right]$$

with

(15) $$v_p = \sqrt{\frac{k \cdot T}{2 \cdot m_p^* \cdot \pi}} = \frac{A_p^* \cdot T^2}{q \cdot N_V}$$

Let us notice that these formulations are also valid for metal-semiconductor Schottky diodes (in that case $\varphi_{na} = \varphi_{pa}$ which is the metal Fermi level).

The expressions of the thermionic currents given here are the components of the currents perpendicular to the surface of the interface and their directions depend on the discontinuities of the conduction band and valence band. At the interface, the thermionic emissions lead to Fermi levels discontinuities.

From a numerical point of view, the thermionic current expressions are used instead of drift-diffusion current formulations in the continuity equations at the interface between two semiconductors.

Presently the finite difference method is used to solve the equations with respect to φ, φ_n and φ_p after linearization (Viallet and Mottet, 1985). The interfaces between two semiconductors are perpendicular to the grid and are located between two nodes. The local mesh refinement corresponds to the interface thickness (some 10 Å). Barrier height lowering under bias depends on the interface thickness.

APPLICATIONS

The results presented in this paper deal with III-V compounds heterojunctions, mainly used in today opto electronics. The layers are *InP* (E_g= 1.35 *eV*) and *InGaAs* (E_g= .75 *eV*) lattice matched to *InP* substrate as those used for 1.5 μm laser diodes and photodiodes. The band discontinuities are ΔE_C= .23 *eV* and ΔE_V= .37 *eV*. In the following three examples, the doping levels are $5 \cdot 10^{15} cm^{-3}$ for *InP* and $5 \cdot 10^{16} cm^{-3}$ for *InGaAs* either *P* or *N type*. The carrier lifetimes used in Shockley-Hall-Read recombination generation term *U*, expressed in Fermi-Dirac statistics (Viallet and Mottet, 1985), are respectively $\tau_n = \tau_p = 10^{-9} s$ in *InP* and $10^{-10} s$ in *InGaAs*.

The first example is an isotype *P-P* heterojunction. Figures 2a and 2b show the .2 V forward bias band diagram and

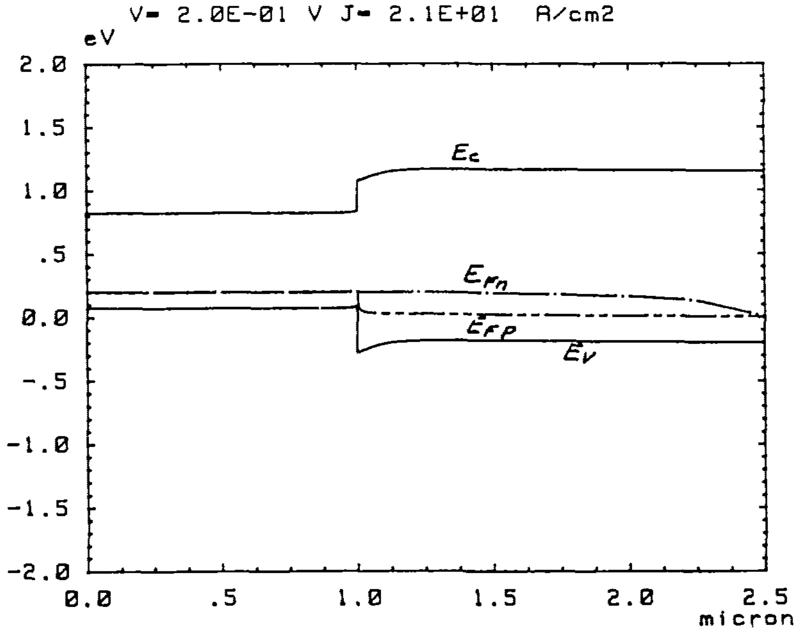

Fig. 2. a) Band diagram of forward bias P - P isotype heterojunction.

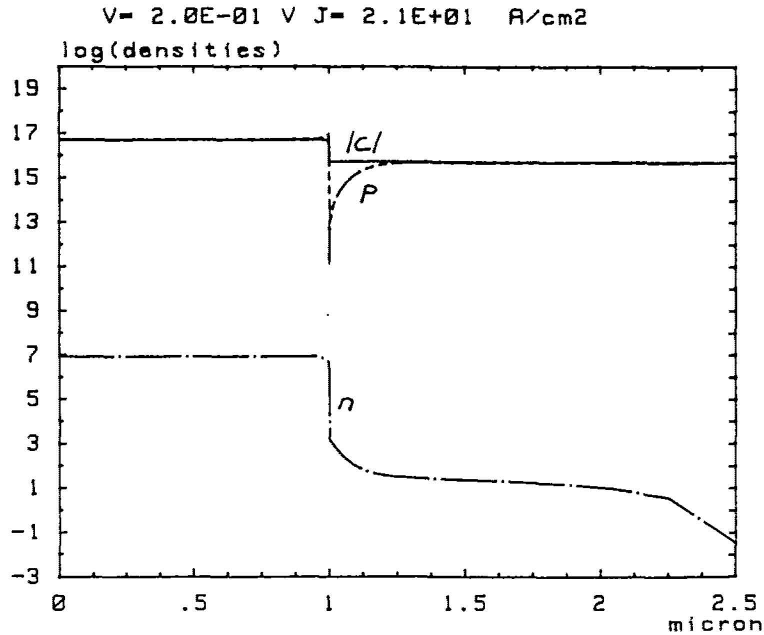

Fig. 2. b) Carrier profiles of forward bias P - P isotype heterojunction.

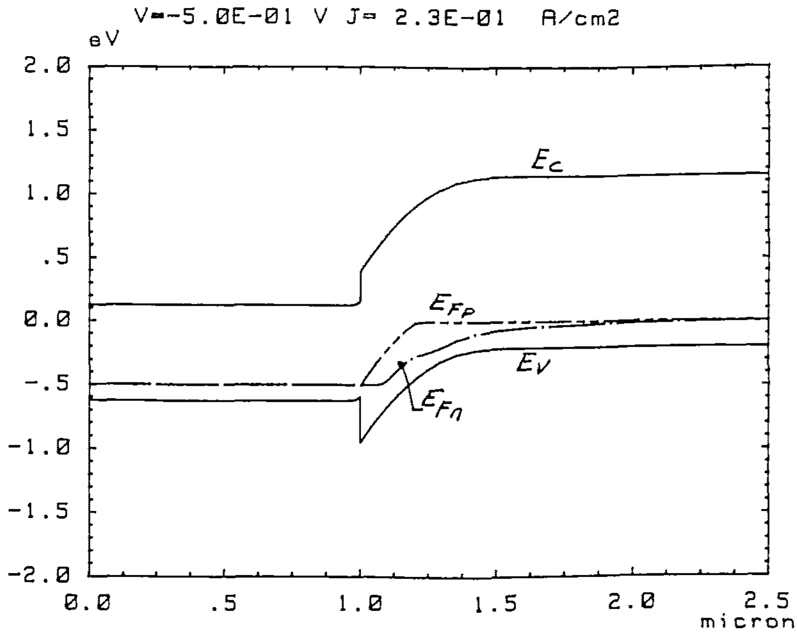

Fig. 2. c) Band diagram of reverse bias P - P isotype heterojunction.

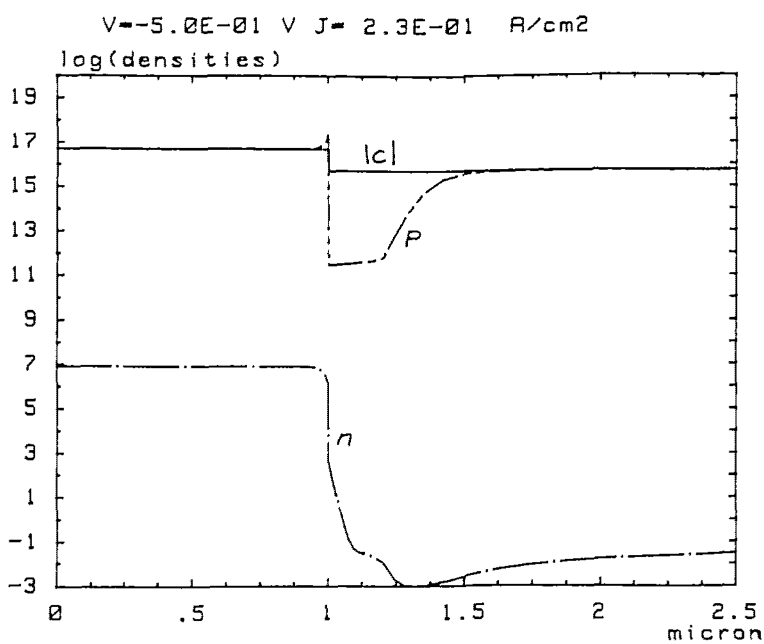

Fig. 2. d) Carrier profiles of reverse bias P - P isotype heterojunction.

carrier density profiles. The hole thermionic emission can be seen on the discontinuity of E_{Fp} at the interface to assure current flowing from *InP* to *InGaAs*. The bending of E_{Fp} close to the heterojunction can be noticed. This effect is due to the limitation of the conduction by the diffusion velocity owing to the low hole mobility in *InP* (150 $cm^2/V/s$) as predicted by the Crowell and Sze (1966) thermionic emission-diffusion theory. In the present case the diffusion velocity is close to the thermal velocity. The exponential behaviour of the forward $I(V)$ characteristics obtained by numerical simulation is in very close agreement with the analytical formulation given by thermionic emission-diffusion theory. Figures 2c and 2d describe the band diagram and density profiles for a reverse bias of -.5V. The space charge region extends only in the *InP* material due to the limitation of the hole thermionic emission from *InGaAs* to *InP*. The reverse current increases with reverse bias due to the increase of the hole carrier density in the *InGaAs* side of the interface, leading to an increase of the p_0 value. The reverse current roughly increases proportionally to the reverse bias.

The second structure is an *N* type *InGaAs* over *P* type *InP* diode. Figures 3a and 3b correspond to band diagram for forward and reverse biases. For the forward bias, the hole termionic emission is clearly seen as the hole Fermi level totally drops at the interface so that there is no extend of the space charge region in *InGaAs*. No drop of the electron Fermi level appears in the figure 3a, even though termionic emission is taken into account. When reverse biased, the space charge region only extends in the *InP*. No hole diffusion occurs in the *N* type material owing to the dominant thermionic emission effect. On the opposite, electrons in *P* type material exibit the standard minority carrier diffusion behaviour of an homojunction diode.

The last structure consists in a *P* type *InGaAs* over *N* type *InP* diode. The behaviour of this diode is quite different from that of the previous case. When forward biased, as shown in figure 4a, the thermionic emission which corresponds to the electron Fermi level drop, is less dominant than for the holes in the previous structure. Diffusion of electrons thus occurs in the *P* type layer. The reason is that the conduction band discontinuity is smaller than that of the valence band. Such a behaviour is confirmed when reverse biasing the diode, as in

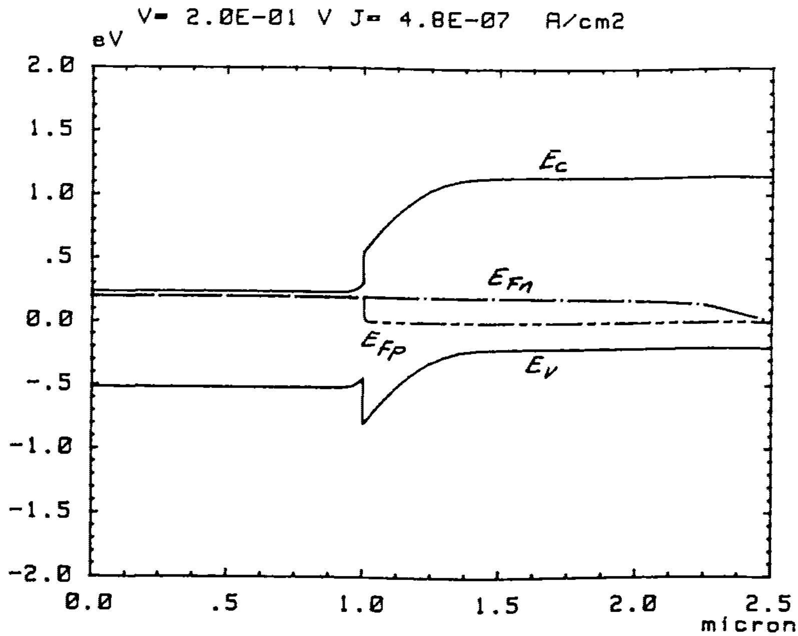

Fig. 3. a) N type InGaAs over P type InP diode under forward bias

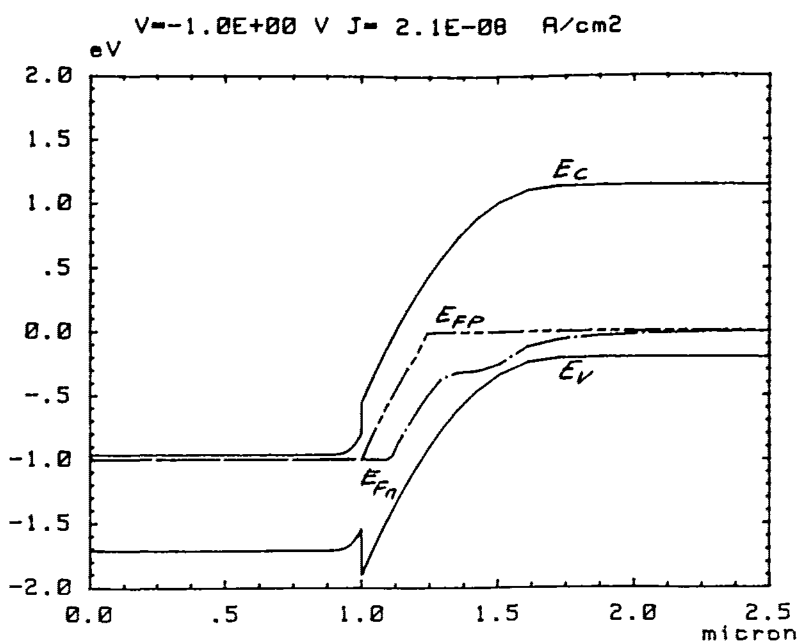

Fig. 3. b) N type InGaAs over P type InP diode under reverse bias

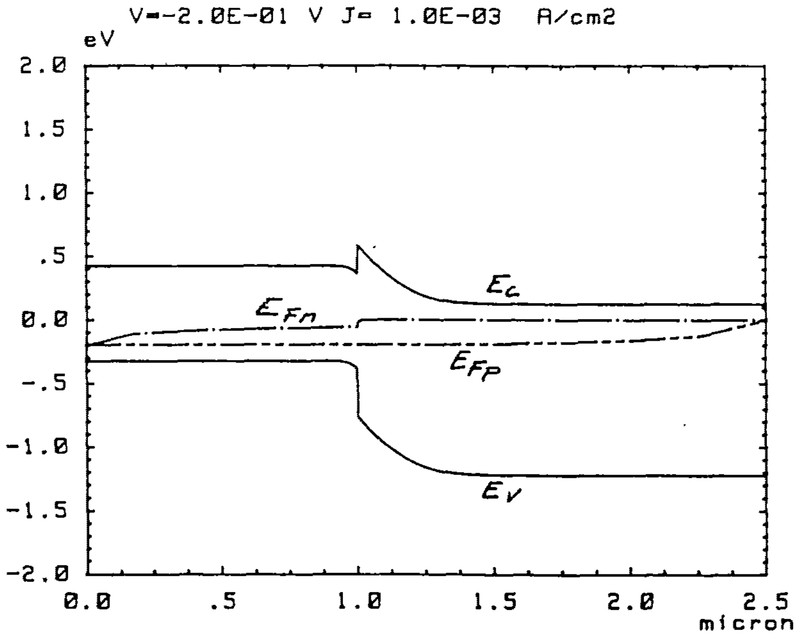

Fig. 4. a) P type InGaAs over N type InP diode under forward bias

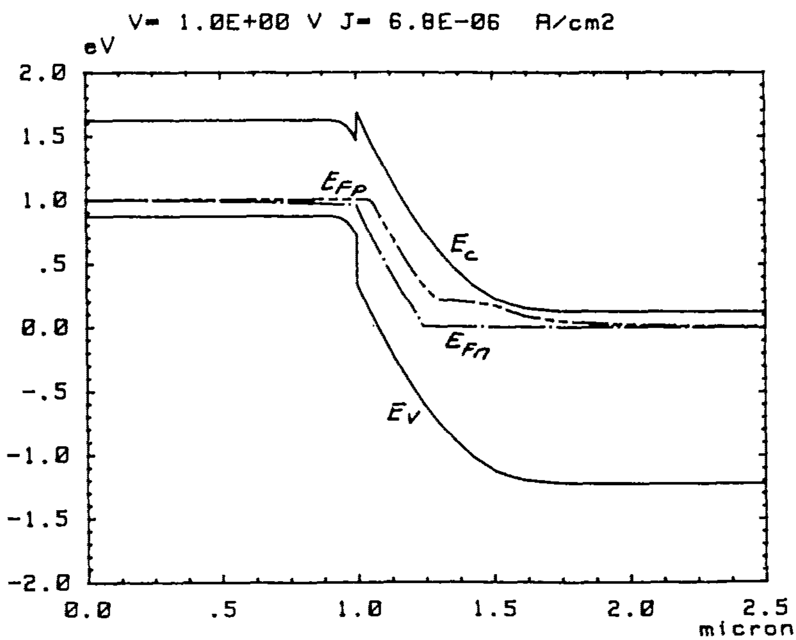

Fig. 4. b) P type InGaAs over N type InP diode under reverse bias

figure 4b, for which the space charge region extends in both layers.

CONCLUSION

A model of thermionic emission at semiconductor heterojunction interface, suitable for the numerical simulation, has been derived. This model is valid for both forward and reverse biases. Examples on both isotype and heterotype III-V heterojunctions stress out the importance of thermionic emission and the behaviour of the different junctions.

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