Negative Differential Resistance in Reverse-Biased Metal-Semiconductor Systems

by

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Abstract—The effect of intervalley carrier transport on the current-voltage characteristics of Au-n-type GaAs metal-semiconductor barriers has been studied theoretically based on the thermionic emission-diffusion theory and the quantum emission-diffusion theory incorporating the Ridley-Watkins-Hilsum mechanism.

A negative differential resistance region is found to exist under reverse-biased condition over wide range of temperature and for dopings below $10^{14}$ cm$^{-3}$. For higher dopings the carrier transport is dominated by field emission as predicted by the quantum emission-diffusion theory. For a Schottky-type Au-GaAs diode with a doping of $10^{14}$ cm$^{-3}$, operated at 373$^0$K, a differential conductance of $-1.5$ m$^2$/cm$^2$ is obtained at a reverse bias of 0.2 V; and for a Mott-type diode with the same doping and an epitaxial layer thickness of 2.4 μm, a conductance of $-2$ m$^2$/cm$^2$ is obtained at 0.3 V.

The average diffusion constant for two-valley system is derived. The result shows considerable departure from the Einstein relation. A discussion is presented concerning the realization of the metal semiconductor system.

1. Introduction

When a metal-semiconductor barrier is formed on a two-valley

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semiconductor such as n-type GaAs, the classical transport analysis of metal-semiconductor systems should be modified to incorporate the Ridley-Watkins-Hilsum (RWH) mechanism [1-3] i.e. the field enhanced redistribution of carriers between the valleys.

In the following analysis, we shall be mainly concerned with n-type GaAs, since it is the most extensively studied two-valley semiconductor. It is well known that in the GaAs band structure there is a high mobility valley (with mobility of about 4000 to 8000 cm²/V·sec) located at the Brillouin zone center, and a low-mobility satellite valley (with mobility of about 100 cm²/V·sec) along the <100> axis, about 0.36 eV higher in energy. The effective mass of electrons are 0.068 m and 1.2 m, in the lower and higher valley respectively; thus the density of states of the upper valley is about 70 times that of the lower valley. When an electric field is applied, the carriers will transport from the higher-mobility low-energy valley to the low-mobility high-energy valley giving rise to a reduction of average mobility with field.

When a reverse bias is applied to the above metal-semiconductor system, the field distribution will change with the applied voltage. This will modify the average mobility and diffusion constant. Increasing of the reverse bias may decrease the diffusion constant which in turn may decrease the current density. Therefore a negative differential resistance is expected in certain field range.

The current-voltage characteristics will be derived in Sec. II for the two valley system based on the thermionic emission-diffusion theory [4] in which the carriers emitted across the barrier maximum are considered. In Sec. III the I-V characteristics are derived based on the quantum emission-diffusion theory [5] in which both the thermionic and tunneling components are considered. A discussion is presented in Sec. IV.

2. Thermionic Emission-Diffusion (TED) Theory

The energy band diagrams of two representative metal-semiconductor barriers under reverse-biased condition are shown in Fig. 1. The only difference between these two barriers is the thickness of the uniformly doped surface layer (or epitaxial layer L) in comparison with the width of the depletion layer W. If L > W, we have the Schottky-type barrier 6; and if L < W, we have the Mott-type barrier. 7.

Consider first the Schottky-type barrier as shown in Fig. 1 (a). The potential profile q\( \phi(x) \) is determined by the electric field associated with the ionized donors and the attractive image force
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experienced by an electron when it approaches the metal. The lowering of the barrier height is \( q\Phi \), and the potential maximum occurs at \( x_m \). The \( \text{imref} - q\Phi_n \) \((x)\) is associated with the current density.

The basic equations for the Schottky barrier are given as:

\[
W = \sqrt{2\varepsilon_s(V_{bi} - V - kT/q)/qN_b}
\]

(1)

\[
E(x) = qN_b(x - W)/\varepsilon_s
\]

(2)

\[
\Psi(x) = qN_b(Wx - \frac{1}{2}x^2)/\varepsilon_s - \Phi_n
\]

(3)

\[
E_m = E(at\ x = 0) = \sqrt{2qN_b(V_{bi} - V - kT/q)/\varepsilon_s}
\]

(4)

where \( W \) is the width of depletion layer, \( \varepsilon_s \) the permittivity, \( V_{bi} \) the built-in potential, \( N_D \) the ionized donor concentration, \( x \) the distance measured from the metal semiconductor interface, \( \Phi_n \) the barrier height, and other symbols have their usual meanings.

The electron current density along the \( x \)-direction is given by

\[
J_n = q\left\{ n(x)\mu_1 \frac{d\Psi(x)}{dx} + \frac{d}{dx}[Dn(x)] \right\}
\]

(5)

where \( n(x) \) is the total electron density, \( \mu \) the average electron mobility, and \( D \) the average diffusion constant of electrons.

In the above expression, the first term is the drift component while the second term is the diffusion component. According to Kroemer’s model \(^8\) the average mobility for GaAs can be expressed as

\[
\tilde{\mu} = \mu_1 (1 + BF^k)/(1 + F^k)
\]

(6)

where for high-purity n-type GaAs at 300K, the parameters in Eq. \( (6) \) are given as follows: \( \mu_1 \) (the low-valley mobility) \( = 8000 \text{cm}^2/\text{V-s} \), \( F = E/(4 \times 10^3) \) with the electric field \( E \) in units of \( \text{V/cm} \), \( k = 4 \), and \( B = 0.05 \).

The electron concentration as a function of distance can be expressed by a Maxwell-Boltzmann distribution:

\[
n(x) = N_C \exp\{-q(\Psi(x) - \Phi_n(x))/kT\}
\]

(7)

where \( N_C \) is the density of states in the lower conduction band, and \( \Psi \) and \( \Phi_n \) are the potential and the \( \text{imref} \) respectively. At zero bias \( J_n = 0 \) and \( \frac{d\Phi_n(x)}{dx} = 0 \).
we obtain
\[
\frac{d\bar{D}}{dx} = q \frac{\bar{D}}{kT} \frac{d\Psi(x)}{dx} - \bar{u} \frac{d\Psi(x)}{dx}
\]  
(8)

from Poisson's equation
\[
\frac{d^2\Psi(x)}{dx^2} = -qN_d/\varepsilon_s
\]

we obtain
\[
\bar{D} = D_1 e^{-r} + \frac{2kT}{E_s^2} r e^{-r} \int_0^E \bar{u}Ee^r dE
\]

(10)

where
\[
D_1 = \frac{kT}{q} u_1 = \text{diffusion constant in lower valley}
\]

\[
r = \frac{\varepsilon_s E_s^2}{(2qN_d kT)}
\]

The variation of D at 3000K with electric field E is plotted in Fig. 2. Also shown is the Einstein relation (dotted line). We note that for dopings lower than 10^15 cm^-3, D follows the Einstein relation at lower fields. As doping or field increases, considerable deviation from the Einstein relation occurs. It can be shown from Eq. 10 that when the temperature is increased, D for a given doping will shift toward higher field. Over a limited field range, however, D can be approximated by
\[
\bar{D} = \frac{kT}{q} \bar{u} = \frac{kT}{q} u_1 (1+BF^k)/(1+F^k).
\]

(10a)

When a reverse bias -V is applied to the metal-semiconductor system, a current flows. Based on the thermionic emission-diffusion (TED) theory [4], the current density can be given as
\[
J_n = -qu_n \frac{d\phi_n(x)}{dx}
\]

(11)

For the region 0 ≤ x ≤ x_m, we assume that it acts as a sink for electrons. We can then describe the current flow in terms of an effective recombination velocity v_R at x_m.
\[
J_n = q (n_m - n_e) v_R
\]

(12)

where n_m is the electron density at x_m when the current is flowing and is given by
\[
n_m = N_e \exp\left(-\frac{q}{kT} \phi_n(x_m) + \phi_B\right)
\]

(13)
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and \( n_0 \) is a quasi-equilibrium electron density at \( x_m \) as given by

\[
n_0 = N_e \exp \left( -\frac{q \phi_n}{kT} \right)
\]

(14)

where \( q \phi_n (x_m) \) is the imref at \( x_m \). Substitution of Eq. 6 into Eq. 11, elimination of \( n \) from Eqs. 7 and 11 and making use of the boundary conditions of Eqs. 13, 14 and

\[
\phi_n(W) = -V
\]

yield the following expression[4]

\[
J_n = \frac{qN_e v_R}{1 + v_R/v_D} \exp \left( -\frac{q \phi_B}{kT} \right) \left[ \exp \left( \frac{qV}{kT} \right) - 1 \right]
\]

(15)

where

\[
v_D = \left\{ \int_{x_m}^{W} \frac{1}{D} \exp \left( -\frac{q}{kT} (\phi_B + \Psi) \right) dx \right\}^{-1}
\]

(16)

is an effective diffusion velocity associated with the transport of electrons from \( x=W \) to \( x=x_m \) and \( D \) is given by Eq. 10a. Figure 3 shows some theoretical results for Schottky-type Au-GaAs barriers with barrier height 0.83 eV and a doping of \( 10^{14} \text{ cm}^{-3} \). The dotted lines are from the TED theory. The solid lines are from the quantum emission-diffusion theory to be considered in the next section. We note that for a given temperature there exists a region in which the differential resistance is negative, i.e. the current decreases as the voltage increases. We also note the strong dependence of the current density on temperature.

We next consider the Mott-type barrier as shown in Fig. 1b. The derivation is basically identical except that the boundary condition at \( x=W \) is replaced by \( \phi_n(L) = -V \). We thus obtain identical expression as Eq. 15 for the Mott-type barrier; the diffusion velocity \( v_D \) is also the same as given by Eq. 16 except that the upper integration limit is replaced by \( L \). The computed results for the Mott type are shown in Fig. 4, which is quite similar to that of Fig. 3. However, at a given temperature and a given bias, the reverse current density for the Mott type is larger by about 30% than that of the Schottky type.

3. Quantum Emission-Diffusion (QED) Theory

According to the quantum emission theory\(^5\) the current transport equation is given by
where $J_{SM}$ is the current density flowing from the semiconductor to the metal

$$J_{SM} = \frac{A^* T}{k} \int_0^\infty V_{bl} - \Delta \phi F_s T(n)(1-F_m) d\eta$$

$$+ \frac{A^* T}{k} \exp\left(-q(V_{bl} - \Delta \phi + V_n)/kT\right) \int_0^\infty \exp(-\zeta/kT) T(\zeta) d\zeta$$

and $J_{MS}$ is the current density flowing from the metal to the semiconductor

$$J_{MS} = \frac{A^* T}{k_c} \int V_{bl} - \Delta \phi F_m T(n)(1-F_s) d\eta$$

$$+ \frac{A^* T}{k} \exp\left(-q\phi_E/kT\right) \int_0^\infty \exp(-\zeta/kT) T(\zeta) d\zeta$$

A* is the effective Richardson constant and $F_s$ and $F_m$ are the Fermi-Dirac distribution functions in the semiconductor and in the metal respectively. $T(\zeta)$ and $T(\zeta')$ are the transmission functions below and above the barrier maximum respectively.

In the TED theory, the contribution of the field emission has been ignored. However in GaAs, the field emission term is much more important than that of Si because of the smaller effective mass in GaAs. From the QED theory for one-valley system (5), the contribution of the tunneling component at 300°K becomes significant at a doping of $10^{15}$ cm$^{-3}$, at higher dopings and lower temperatures, tunneling will become even more important.

In the QED theory for two-valley system the following assumptions are made: 1. there is no interaction between the quantum emission and the diffusion mechanism, 2. the total current is determined by the combined conductance of two series conductances resulting from the above two mechanisms, and 3. the diffusion mechanism occurs. only within the range from the emitted band edge to the barrier minimum. According to the assumptions 1 and 2, we obtain for the total current density:

$$J = \frac{J_{QE} J_D}{J_{QE} + J_D}$$

where $J_{QE}$ is the quantum emission current and $J_D$ is the diffusion current. The diffusion velocity is given by Eq. 16 in which the diffusion constant is given by Eq. 10 and the lower limit of integration in Eq. 16 is replaced by $x_E$ which is the position at
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which the maximum amount of carrier transport occurs [9]:

\[ x_E = W \left(1 - \cosh^{-1}\left(\frac{1}{RT}\right)\right) \] (21)

and

\[ R = \sqrt{4m^*\varepsilon_s/\hbar^2N_0} \]

Since the ratio of \( J_{QED} \) and \( J_D \) can be approximated by the ratio of the recombination velocity and diffusion velocity [4], we obtain from Eq. 20

\[ J = \frac{J_{QED}}{(1 + v_R/v_D)} \] (22)

It is thus obvious that when \( x_E \) equals zero, the result will automatically reduce to that of the TED theory [4]. However, when tunneling becomes more important, \( x_E \) will occur at a lower band edge. When \( T/N_D \) tends to zero (i.e. tunneling dominates) \( x_E \) approaches \( W \) and thus the diffusion mechanism becomes less important.

The theoretical results based on the QED theory are also shown in Fig. 3 and 4 (solid lines) for Schottky-type and Mott-type barriers respectively. We note that at small reverse voltages, the results are identical to that obtained from the TED theory. At larger voltages, however, the current will increase because of field-emission processes. Figure 3(b) shows the doping effect on the reverse I-V characteristics. It shows that as the doping decreases, the negative differential resistance region occurs at higher reverse voltages (e.g. >3 V at 10^{13} cm^{-3}, and >30 V at 10^{12} cm^{-3}).

4. Discussion

The current-voltage characteristics of metal-semiconductor systems formed on two-valley semiconductors have been considered theoretically. Both the TED theory and QED theory predict the existence of negative differential resistance over certain field range. The QED theory is believed to be more accurate since it takes into account the thermionic and tunneling current components.

In quantum emission-diffusion theory, the negative differential conductance will occur only for samples with doping concentration equal to less than 10^{14} cm^{-3}. The maximum differential negative conductance occurs at about 0.1 V and reaches a minimum at 0.2 V. For lower dopings the position of the maximum differential
conductance shifts toward higher voltages, while for higher dopings it shifts toward lower voltages. At even higher dopings, the negative conductance will not exist due to tunneling which smears out the intervalley transport effect. The tunneling mechanism will also play an important role at large reverse biases at which the current will start to increase rapidly.

In Fig. 3 and 4, as the temperature decreases, the statistical probability decreases (e.g. Boltzmann distribution function), both the free carrier concentration and the diffusion constant also decrease. Thus the total current density decreases as can be seen in the figures.

The bias effect of I-V characteristics is mainly due to the field dependence of electron mobility and the bias dependence of electron concentration. As the reverse bias increases from zero, the current due to majority carrier injection dominates over the decrease of the field-enhanced diffusion velocity. As the bias is further increased, the field-enhanced diffusion velocity becomes more effective, thus a negative differential resistance is observed. In Mott-type barrier, one can choose a suitable $N_D$ and $L$ such that the electric field can be confined within the range $3 \times 10^3 \text{ V/cm}$ to $2 \times 10^4 \text{ V/cm}$ in order to make the reduction of the diffusion velocity more effective. However, in Schottky-type barrier, this condition can not be filled because it always contains the ineffective field region from zero to $3 \times 10^3 \text{ V/cm}$. This can well explain the larger negative differential conductance observed in Mott-type barrier.

In order to realize the metal-semiconductor system with negative differential resistance, it is necessary to improve the material technology of two-valley semiconductors, so that dislocation density and defect centers can be reduced; and doping uniformity across the sample can be maintained. It is also necessary to eliminate the edge effect (e.g. by the use of a diffused guard-ring structure [10]) so that the leakage current can be minimized.

References
3. For a review on the bulk-effect devices associated with the RWH mechanism see, for example, S. M. Sze, "Physics of
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7. N. F. Mott, "Note on the Contact between a Metal and an Insulator or Semiconductor". Proc, Camb. Phil. Soc., 34, 568 (1938).


(a) SCHOTTKY-TYPE BARRIER

(b) MOTT-TYPE BARRIER
Fig. 2. Field enhanced diffusion constant versus field in GaAs.
Fig. 3. Reverse I-V Characteristics of Schottky-type Au-GaAs barrier 
(a) $N=10^{14}$ cm$^{-3}$
Fig. 3. Reverse I-V characteristics of Schottky-type Au-GaAs barrier.

(b) $N=10^{12}, 10^{13}$ cm$^{-3}$
Fig. 4. Reverse I-V characteristics of Mott-type Au-GaAs barrier.
Fig. 5. Negative differential conductance versus voltage for Au-GaAs metal-semiconductor barriers.