1995

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(Received 25 July 1994; accepted for publication 15 December 1994)

A simple one-speed solution to the Boltzmann equation is used to evaluate the mobility and diffusion coefficient for carriers in forward-biased semiconductor barriers. The analysis shows that although the average kinetic energy of carriers remains near thermal equilibrium, the mobility and diffusion coefficient are strongly reduced by the built-in field. Conventional macroscopic transport equations, which treat the carrier mobility and diffusion coefficient as single valued functions of the kinetic energy will improperly treat transport in forward-biased barriers. The results are important for the careful analysis of metal–semiconductor and heterojunction diodes. © *1995 American Institute of Physics.*

Metal–semiconductor (MS) and semiconductor heterojunction diodes are conventionally analyzed by describing carrier transport in the barrier with a drift-diffusion equation then imposing a thermionic/field emission boundary condition at the junction.[1–3] The problem of specifying the carrier mobility to use within a forward-biased barrier has been unresolved since Gunn first raised the issue in 1968.[4] Gunn concluded that one should use the high-field, bulk mobility in the barrier, but his analysis ignored carrier diffusion by assuming a specific perturbing potential which would not appear to occur in practice. Subsequently, most workers have used the low field, bulk mobility (e.g., Ref. 5), but some use the high field, bulk mobility (e.g., Ref. 6). Numerical simulations of MS and heterojunction diodes, however, demonstrate that the current-voltage characteristic depends on the assumed mobility,[6,7] so it is important to resolve this issue. In this letter, we use a simple one-speed solution to the Boltzmann equation to demonstrate that although the average kinetic energy of carriers within the forward-biased barrier is very near $3kT/2$, the carrier mobility is strongly reduced by the field.

One might expect to use a field-dependent mobility within the barrier because the electric field is high. In a bulk semiconductor, the electric field heats the carriers, which degrades the mobility, but in a forward-biased barrier, the net flow of carriers is against the field, so carriers are cooled rather than heated.[8] Detailed numerical solutions of the Boltzmann equation for a semiconductor heterojunction show that the carrier energy is very near 3/2 kT throughout the barrier, except for the kT layer (the region near the junction where the potential drops by kT/q),[9] where some cooling occurs.[10] For these reasons, it has been common practice to use the low-field mobility within a barrier, but it is easy to demonstrate that this is incorrect.

Consider the simple Mott barrier sketched in Fig. 1 (a Mott barrier has a constant electric field in the barrier). If we integrate the drift-diffusion equation for the carrier flux,

$$F=-n\mu_n E-D_n\frac{dn}{dx}, \tag{1}$$

across the barrier subject to the boundary conditions, $n(0)=F/v_T$ and $n(-W)=N_D$, we find,

$$F=\frac{N_C v_T}{(1+v_T/\mu_n E)}e^{-q\varphi_{Bn}/kT}e^{qV_A/kT}. \tag{2}$$

We have assumed the Einstein relation and the mobility is constant at μ_n, with its value in a bulk semiconductor under low field. We also assumed that the velocity distribution is hemi-Maxwellian at $x=0$, so the average x-directed velocity is $v_T=\sqrt{2kT/\pi m^*}$, which is twice the so-called Richardson velocity, v_R. For high electric fields, the flux should be given by the thermionic emission theory as, $F=N_C v_R e^{-q\varphi_{Bn}/kT}e^{qV_A/kT}$, but Eq. (2) reduces to a value, that is a factor of 2, too large. [It is worth noting, however, that if one follows common practice and uses a physically incorrect boundary condition of $n(0)=F/v_R$, the correct final result is obtained. This point has been discussed by Berz.[9]]

McKelvey's flux method[11] provides a one-speed solution to the Boltzmann equation that can be used to evaluate the carrier mobility with the forward biased barrier. Consider a slab of thickness dx with left- and right-directed fluxes as

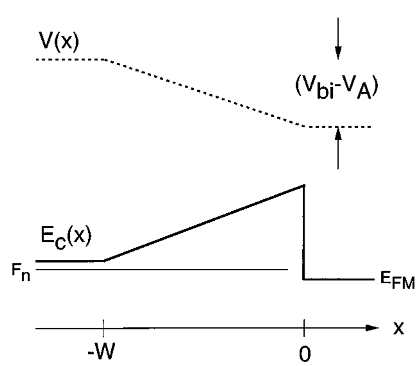

FIG. 1. The conduction band and electrostatic potential profiles for a simple Mott barrier. (A Mott barrier is one in which the electric field is constant.)

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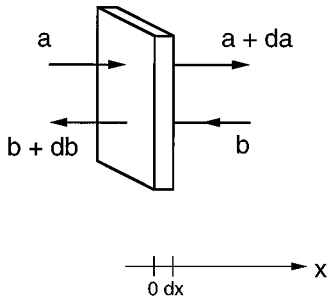

FIG. 2. Definition of the carrier fluxes for McKelvey's flux method. The right-directed fluxes are denoted by a and $a+da$, and the left-directed fluxes are b and $b+db$. Each flux is taken from the positive or negative half of a thermal equilibrium Maxwellian velocity distribution.

shown in Fig. 2. We assume an electric field in the $-x$ direction, so that left-directed electrons experience a potential barrier. We further assume that the left- and right-directed fluxes are taken from the positive and negative halves of a thermal equilibrium Maxwellian velocity distribution. The overall carrier distribution function, therefore, varies from a full Maxwellian at $x=-W$ to a hemi-Maxwellian at $x=0$, if we neglect backscattering at the junction. More detailed, numerical simulations confirm that these are reasonable assumptions in a forward-biased barrier.[10,12,13]

Assuming backscattering coefficients of ζ for the left-directed flux and ζ' for the right-directed flux, we have

$$\frac{da}{dx}=-\zeta a+\zeta' b=\frac{db}{dx}. \tag{3}$$

Noting that the carrier density and flux are given by $n(x)=a(x)+b(x)/v_T$ and $F=a(x)-b(x)$, we can reexpress Eq. (3) as

$$F=\frac{(\zeta'-\zeta)}{(\zeta'+\zeta)}v_T n(x)-\frac{v_T}{(\zeta'+\zeta)}\frac{dn}{dx}. \tag{4}$$

The flux equations, which are valid for both ballistic and diffusive transport[11,14] and which do not assume an overall Maxwellian distribution, can be expressed in drift–diffusion form if we define the mobility and diffusion coefficient as

$$\mu=\frac{(\zeta'-\zeta)v_T}{(\zeta'+\zeta)\,E} \tag{5a}$$

and

$$D=\frac{v_T}{(\zeta'+\zeta)}. \tag{5b}$$

To derive the field-dependent mobility and diffusion coefficient, the backscattering coefficients must be specified. For the flux flowing down the potential barrier, ζ' should be the same as the backscattering coefficient for a bulk semiconductor in equilibrium. This is so because the injected flux is nearly an equilibrium half-Maxwellian and as long as the potential drop across the slab is $\ll kT/q$, it can have little effect on backscattering. As a result, we find[14]

$$\zeta'=\frac{v_R}{D_n}, \tag{6a}$$

where $D_n=(kT/q)\mu_n$ is the low-field, bulk diffusion coefficient.

For the flux that flows against the barrier, however, we have to be more careful. The backscattering coefficient for this flux can be written as

$$\zeta=1-(1-\zeta')e^{-q\Delta V/kT}, \tag{6b}$$

where ΔV is the potential drop across the slab. For ballistic transport, Eq. (6b) is simply the thermionic emission result.[14] When scattering occurs, however, the thermionic emission result is modified using Price's detailed balance argument.[15] Using Eqs. (6) in Eq. (5b), we find

$$D=\frac{1}{\frac{(1-e^{-q\Delta V/kT})}{v_T dx}+\frac{(1+e^{-q\Delta V/kt})}{2D_n}}, \tag{7}$$

which, assuming the slab is thin, $\Delta V\ll kT/q$, reduces to

$$D=\frac{D_n}{1+E/E_{cr}}, \tag{8}$$

where

$$E_{cr}=v_T/\mu_n. \tag{9}$$

By similar arguments, we find

$$\mu=\frac{\mu_n}{1+E/E_{cr}}, \tag{10}$$

where μ_n is the bulk, low-field mobility. When these field-dependent transport parameters are used in the drift-diffusion equation, the correct current–voltage characteristic for the Mott barrier results [i.e., Eq. (2) with v_T replaced by v_R].

Equations (8)–(10) show that the mobility and diffusion coefficient are field dependent in a forward-biased barrier. We have assumed near-equilibrium left- and right-moving fluxes, so the field dependence is not associated with hot carrier effects. The equilibrium Einstein relation is obeyed, and the critical field is related to the thermal velocity, not to the saturated velocity. Because of the high electric field, there is a steep concentration gradient, and a field-dependent D results to limit the diffusion velocity to v_T.[15] Because the Einstein relation holds, there is a corresponding reduction in μ. Finally, it is interesting to note that the drift–diffusion equation can also be expressed as

$$J_n=n\mu(E)\nabla F_n^*, \tag{11a}$$

where

$$F_n^*\equiv E_C+kT\,\ln(n/N_C). \tag{11b}$$

Equation (11) applies in the barrier, even in the kT layer where the deviations from equilibrium are typically very large. Near equilibrium, where the carrier distribution is nearly Maxwellian, F_n^* reduces to the quasi-Fermi level, but F_n^* is defined by Eq. (11b), even for highly non-Maxwellian distributions.

In conclusion, we have shown that carrier transport in a forward-biased semiconductor barrier can be described by a drift–diffusion equation, but the mobility and diffusion coefficient are strongly reduced by the built-in electric field. The reduction in D occurs to limit the maximum diffusion velocity to v_T in the presence of the strong concentration gradient induced by the built-in field. This occurs despite the fact that the average kinetic energy remains very near its equilibrium value of $3kT/2$. As a consequence, conventional macroscopic transport models which treat the carrier mobility as a function of the carrier kinetic energy or temperature, will improperly treat semiconductor barriers. The result of improperly specifying the mobility is a factor of two or so error in the computed current, which corresponds to a fairly small change in the effective barrier height of $\approx kT$, but the effect should be considered for accurately modeling metal-semiconductor and heterojunction diodes. Finally, we note that our analysis is based on the assumption that the distribution function can be described by two differently weighted halves of a thermal Maxwellian velocity distribution. Numerical techniques, like those reported in Ref. 10 must be used to treat the modest cooling that occurs in the kT layer.

One of the authors (M.L.) thanks S. Luryi for pointing out that similar conclusions can be reached by using the concentration-dependent diffusivity introduced in Ref. 15. The work at Purdue University was supported in part by the MRSEC Program of the National Science Foundation under Award No. DMR-9400415.

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