Energy Oscillations in Electron Transport Across a Triangular Barrier

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Abstract—Carrier transport across the semiconductor space-charge region of a silicon triangular barrier diode is investigated by a Monte Carlo simulation. Oscillations of the electron mean kinetic energy are observed as a function of position along the uphill slope of the barrier under bias. At a given point on the uphill slope, the energy distribution function also shows an oscillatory behavior, with a periodicity corresponding to the optical phonon energy. These oscillations are shown to be due to the nonequilibrium dynamics of the electron interaction with optical phonons in the situation when other inelastic electron scattering processes are negligible. The energy oscillations are superimposed on a smooth cooling of the distribution in the transport toward the top of the barrier, as current flows through the system. Comparison with the thermionic theory quantifies the importance of nonequilibrium effects in short-range electronic transport.

I. INTRODUCTION

Modern technology allows the fabrication of the so-called "mesoscopic structures" whose characteristic dimensions (≈ 0.1 μm) are in the range between the microscopic atomic scale and the scale of conventional macroscopic systems (≥ 1 μm). A number of interesting mesoscopic phenomena of quantum-mechanical nature arise when the system size is comparable to the coherence length of electronic wave functions. Interesting mesoscopic effects arise also in classical electron transport. Such effects can be expected when the size of the system is less than a characteristic length associated with certain scattering processes. A well-known example of a classical mesoscopic effect is the velocity overshoot [1].

The purpose of this paper is to present an accurate Monte Carlo (MC) analysis of the classical electron transport in a mesoscopic triangular barrier (TB) diode. Rectifying TB diodes have been first demonstrated experimentally in planar-doped-barrier (PDB) structures [2] and graded-gap heterostructures [3]. We shall restrict our attention to the PDB version of a TB diode. The PDB [n-i-δ(p⁺-i)-n] structure consists of a nearly intrinsic layer (i) of thickness L sandwiched between two n-type low-resistivity layers. In the process of crystal growth a p⁺-doped region of thickness δ ≪ L and doping N⁺ is built into the i region. Acceptors in the p⁺ layer are completely ionized forming a negative charge sheet of surface density Σ = qN⁺δ which gives rise to a triangular potential barrier with shoulders L₁ and L₂ and height Φ (see Fig. 1 for a schematic of the structure) approximately given by [2]

\[ \Phi = -\frac{\Sigma L_1 L_2}{e L}. \]

Theoretical studies of transport in TB diodes have included the effects of carrier diffusion into the undoped (i) layer [4] that modify the above expression for Φ and strongly affect the current-voltage characteristics, as well as bipolar effects [5] that become important when the barrier height Φ is comparable to the semiconductor bandgap. Analytical expressions [6] for the current-voltage characteristics of the TB structure give a reasonable agreement with experimental results. However, these expressions have been obtained from considerations based on the drift-diffusion equation; the important effects of carrier acceleration and heating have been included only crudely, through a thermionic model of barrier transport. A more refined treatment was used by Cook [7] who coupled an energy flow equation to the drift-diffusion (DD) model and performed calculations on PDB's. The carrier acceleration effects are naturally included in an MC analysis. Previous MC studies [8], [9] of planar-doped GaAs diodes have found significant enhancement in the electron velocity on the downhill slope due to the effects of ballistic transport and velocity overshoot. These nonequilibrium effects, not accounted for by the DD model, dominate the transient characteristics of GaAs TB diodes upon a sudden change in bias [9]. The present work was set out to investigate similar effects in silicon. In particular, we were interested in the velocity overshoot and ballistic transport on the downhill slope of the TB, expected to enhance the overall barrier conductivity. The first surprise of this investigation was the result that MC calculations consistently predicted a lower current than that predicted by accurate numerical solutions of the DD equation at the same bias (and virtually the same uphill barrier...
height). This observation is explained by a smooth cooling of the carrier distribution in the uphill transport toward the top of the barrier, an effect already predicted theoretically by Stratton [10].

Another interesting result of the present work is the observation of oscillations in the mean kinetic energy of electrons as a function of the position along the barrier. At a given point on the uphill slope, the energy distribution function also shows an oscillatory behavior. These oscillations have the periodicity related to the optical phonon energy and reveal an important peculiarity of the mesoscopic transport. Our main results will be presented in Section III, following the description (Section II) of the algorithms used. Comparison of our MC results with the standard thermionic approach to the barrier transport is briefly discussed in Section IV, where we identify a conceptual error in interpreting the values of both the velocity and the concentration of carriers within the thermionic model. Section V discusses the relation of our present results with other recent studies of classical mesoscopic transport and summarizes our conclusions.

II. THE MONTE CARLO MODEL

The Monte Carlo method applied to charge transport in semiconductors [11] is used to solve the Boltzmann equation by simulating a large number of carriers subject to external forces (electric field) and given scattering mechanisms. In order to adequately study the injection of carriers over a potential barrier, we must solve the problem of simulating rare events such as an electron reaching the top of the barrier. In fact, the probability of an electron to overcome the barrier decreases exponentially with the barrier height. In our case of a TB device with typical values of $\Sigma/q \approx 10^{12}$ cm$^{-2}$ [2], the potential barrier can be as high as $15kT/q$ depending on bias conditions. Such a barrier leads to a drop in the carrier concentration along the uphill slope by more than five orders of magnitude. Such a drop cannot be handled by standard MC techniques, especially if a large amount of statistics is needed at the top of the barrier.

In order to avoid spending an impractical amount of computer time, previous MC studies have either limited the maximum barrier height to three times the thermal voltage [12], or used an algorithm which, in our opinion, neglects certain interesting details of carrier transport in the uphill region of the TB device [9]. The flux of electrons across the barrier arises from two different contributions: high-energy electrons thermally generated in the n$^+$ cathode and propagating uphill without much energy loss, and those which gain energy absorbing optical phonons along the uphill slope. The former group can only be important for ultra-narrow TB's, with shoulders shorter than the mean-free path for optical phonon emission. The second group, of particular interest for the purpose of this paper, is almost neglected in [9], since the statistical enhancement is performed only at the injection contact. In order to overcome this problem, we used two different approaches to the MC algorithm aimed at increasing the statistics of rare events.

The first approach is a modification of that proposed by Phillips and Price [13]. Electrons are distributed over the entire device uniformly, but because of the electric field, they leave the barrier region quickly, and with a multiplication technique these regions can be repopulated so as to maintain adequate statistics everywhere.

The second approach uses the Weighted Monte Carlo algorithm [14], which generates probabilities of the free-flight duration, the scattering events, and the states after scattering in such a way that electrons are "guided" to regions of the $(r,k)$ space that are of a particular interest. In our case we have forced the electrons to surmount the potential barrier even at small applied bias, by favoring the absorption of optical phonons over their emission and small angles with the direction of the external applied field.

The two methods, when applied to the TB device, gave the same results, thus reassuring about their validity.

The silicon model used in our MC simulations has been described in [15]. The scattering mechanisms included are inelastic optical phonons, inelastic acoustic phonons (important to account for the energy exchange with the lattice by low-energy electrons), and ionized impurity scattering. Electron-electron interaction has been neglected because of the low electron density in most the barrier layer.

The considered structure featured a length of 0.3 $\mu$m, containing two $n^+$ regions, 0.05 $\mu$m long and doped to $10^{18}$ cm$^{-3}$, and in the middle a $p^+$ sheet of charge $\Sigma/q = 9.5 \times 10^{11}$ cm$^{-2}$. The resulting equilibrium potential energy barrier is symmetric with $\Phi = 0.71$ eV and extends 0.1 $\mu$m on each side. Both the uphill and downhill slopes correspond to an electric field of $7 \times 10^4$ V/cm. Fig. 1 shows a schematic band diagram of the structure; because of its symmetry there is no difference between "forward" or "reverse" bias and the current direction can be chosen arbitrarily.

III. ENERGY OSCILLATIONS

We have simulated the transport behavior of the system at different applied voltages. For each bias the potential distribution has been self-consistently calculated with a Poisson solver [16]. Fig. 2 displays the potential barrier and the electron kinetic energy as a function of position for applied voltages of 0.7, 0.8, and 1.3 V. If the applied bias is not too high (0.7, 0.8 V), the potential is approximately given by the sum of the equilibrium potential and that due to a constant external field. For higher biases (e.g., at 1.3 V) the potential in the uphill region is distorted (see Fig. 2(c)) because of the space-charge effects [4, 6].

The most interesting feature of the results shown in Fig. 2 is the presence of oscillations in the electron mean kinetic energy, observed along the uphill slope of the barrier for every bias condition. The distance between successive peaks corresponds to a change of potential energy equal to the energy of an optical phonon. This indicates that the oscillations originate from the interaction of electrons with the field of optical phonons.

To better understand the physical process that leads to the spatial oscillations in electron mean kinetic energy, we have performed a simplified simulation with only the uphill slope of the barrier included. Electrons generated at the bottom of the barrier are allowed to move up towards the barrier top. When an electron is scattered back to the starting point, it is specularly reflected, and those electrons that go over the top are taken away from the simulation. In this case we have simulated only 500 $\AA$ of the uphill slope and we checked that the obtained results are not influenced by this simplification.

Electrons entering the barrier from the left with a thermal energy $KT$ can move uphill to a position where the potential energy is of the order of $KT$, and in doing so they lose their kinetic energy. Electrons, however, can exchange energy with the lattice by multiples of the optical phonon energy (for simplicity, we neglect the inelastic acoustic scattering in this ar-
For a given electron, let $\delta n$ be the difference between the number of absorption and emission events it suffers. Electrons may reach higher positions in the barrier as $\delta n$ increases above zero. Substantially above the thermal energy, only electrons with $\delta n > 0$ are present and their kinetic energy contribution decreases as they move uphill. Consider an electron that starts to climb the barrier with a kinetic energy $KT$. The farthest it can go without absorbing a phonon (i.e., staying in the population with $\delta n = 0$) is the point with the potential energy $KT$, where its contribution to the total kinetic energy is zero. Immediately beyond this point the mean kinetic energy must increase because electrons with $\delta n = 0$ are no longer present, and then it decreases again as the remaining electrons lose their kinetic energy in climbing the barrier. Similar considerations apply to electrons with $\delta n = 1$ that can reach up to a point with potential energy $K + h\omega$, where $h\omega$ is the optical phonon energy (51 meV in our model), to electrons with $\delta n = 2$, etc. Such a simple reasoning leads to peaks in the mean kinetic energy at positions corresponding to potential energies just above $KT, K + h\omega, K + 2h\omega, \ldots$.

The actual picture is somewhat more complicated. Because of the energy dependence of the electron–phonon scattering cross section, the contribution to the kinetic energy of electrons with, say, $\delta n = 1$, is maximum at a position where the potential energy is somewhat higher than $K + h\omega$. Fig. 3(a), corresponding to $V_{\text{app}} = 0.8$ V, shows the separate contributions to the mean kinetic energy from electrons with $\delta n = 0, 1, \ldots$ as a function of position. (We define the contribution to the mean kinetic energy of a family as the sum of the kinetic energies of all electrons in that family divided by the total number of electrons at a given point of the barrier). It can be seen that the contributions of the different families of electrons with $\delta n = 0, 1, \ldots$ to the total kinetic energy show peaks which are located near positions with potential energies $0, h\omega, 2h\omega, \ldots$. As seen from Fig. 3(b), the largest contribution to the first maximum results from electrons with $\delta n = 0$ and $\delta n = 1$, the second maximum is mainly built from electrons with $\delta n = 1$ and $\delta n = 2$, and so on for the other maxima. At room temperature, the shape of each electron family is such that the maximum of total kinetic energy is located between two maxima of successive families. At lower temperatures, instead, the individual contributions from the electron families with different $\delta n$ are much narrower and hence better resolved. Accordingly, in this case the maxima of kinetic energy are positioned over each separate contribution.

So far, we have neglected acoustic phonon scattering that is responsible for the "fine structure" of the thermalization in an equilibrium system. However, electrons stay in the TB region for only a short time and cannot be thermalized by acoustic phonons, which are characterized by small energy exchanges and low scattering rates. This assertion is supported by two additional observations: if we look at the differences between Fig. 2(a), (b) and Fig. 2(c), we see that the peaks are more pronounced for the smallest applied bias, i.e., when the retarding electric field is higher and the average permanence time of the electrons in the barrier is smaller. In fact, the stronger is the retarding field the sooner most of the electrons are rejected back to the highly doped region. Furthermore, it can be seen from Fig. 2(c) that in the part of the uphill slope, that has been flattened because of the strong applied potential, the energy oscillations are totally destroyed and this is due to the longer time that electrons spend in this region.

To clarify the roles played by both optic and acoustic phonons in the generation and the smoothing of the kinetic energy oscillations, we have performed several additional experiments. Thus Fig. 4 displays the results obtained neglecting optical phonons but retaining the inelastic acoustic phonon scattering: in this case, the oscillations are seen to disappear. Conversely, if only optical phonons are retained, the oscillations increase in magnitude without changing the peak positions (Fig. 5).

The role of acoustic phonons in momentum relaxation cannot be neglected, in general. However, in the thermionic regime, when the uphill slope is steep, even that role is not essential.
Fig. 3. (a) Contribution to the mean kinetic energy of the different populations of electrons. (b) Mean kinetic energy (dotted-dashed line) and partial sums of different populations. The solid line is the sum of populations with \( \Delta n = 0 \) and \( \Delta n = 1 \), the dashed curve is the sum of populations with \( \Delta n = 1 \) and \( \Delta n = 2 \), the dotted curve is the sum of populations with \( \Delta n = 1 \) and \( \Delta n = 2 \). The horizontal axis shows the distance from the bottom of the barrier.

Fig. 4. Mean electron kinetic energy for \( V_{eq} = 0.8 \) V. The simulation is performed neglecting the interaction with optical phonons but retaining the inelastic acoustic scattering.

This is evident from the fact that the electron mobility does not enter Richardson's formula. Acoustic phonons become important only in the diffusion limit, corresponding to gentle uphill slopes.

At equilibrium, when no current flows across the TB, there can be, of course, no oscillations. Obviously, we cannot describe the equilibrium case focusing only on particles entering the barrier from one side. At each position a perfect balance must be maintained between electrons going uphill and downhill. This balance not only produces a zero current but also guarantees a mean electron kinetic energy exactly equal to \( \frac{3}{2} kT \) everywhere. When a current flows, one of the two fluxes dominates and the balance is broken. When the balance is broken in favor of the uphill flux, the interaction with optical phonons not only leads to the spatial oscillations of the electron mean kinetic energy, but also to oscillations in the electron energy distribution at any point of the uphill slope. Fig. 6 shows the
energy distribution function at two different positions in the device. In the highly doped region, Fig. 6(a), the distribution function is Maxwellian. In contrast, the distribution function on the uphill slope, Fig. 6(b), shows oscillations that are superimposed on the Maxwellian curve and have the periodicity corresponding to the optical phonon energy.

The physical origin of the periodic oscillation in the distribution function at a given point of the uphill slope will be discussed at the end of the next section.

IV. DISTRIBUTION FUNCTION AT THE BARRIER TOP

Fig. 7(a), (b) shows the electron velocity and energy distribution functions at the top of the barrier for $V_{app} = 0.8$ V. The velocity distribution is asymmetrical because most of the injected electrons do not come back. This situation is quite similar to that for a forward-biased Schottky-barrier diode [12]. However, in contrast to the Schottky-barrier case, the distribution function is not exactly hemi-Maxwellian because some electrons do return from over the cliff in the TB. In Fig. 7(a) the tail on the negative side of the velocity axis represents carriers scattered back into the retarding field region.

The nonequilibrium distribution displayed in Fig. 7, corresponds to a depressed ($= 270$ K) electron temperature (defined as the inverse of the slope of the logarithm of the electron energy distribution). This indicates that the electronic system cools off in the transport toward the top of the barrier. Such an effect has been predicted by Stratton [10]. Reduction of the electron temperature is due to the work that electrons perform against the electric field in order to reach the barrier top. This effect is exactly the opposite to the electron heating that takes place on the downhill slope, where electrons are driven by the field.

The electron cooling effect arises due to the high retarding field present in the TB device. Such an effect must also occur in more conventional devices with high retarding fields. The fact that it was not noticed in the MC modeling of a forward-biased Schottky diode [12] is probably due to a low value of the barrier height assumed in that simulation. This nonequilibrium effect tends to disappear at higher applied biases (i.e., weaker retarding fields), when the electron effective diffusion velocity on the uphill slope [6] approaches the equilibrium thermionic emission velocity $v_{th}$.

In this connection it may be worthwhile to point out a common misconception in the interpretation of the thermionic emission theory. It is customary [18] to interpret the Richardson expression for the thermionic current in terms of the product of the equilibrium carrier concentration at the top of the barrier and the so-called "effective recombination velocity" $v_{rec} = (KT/2\pi m^*)^{1/2}$ (at room temperature, for a barrier on a (111) Si surface, $v_{rec} = 5 \times 10^6$ cm/s). These quantities, however, do not correspond to the real concentration and the real velocity of carriers at the top of the barrier. Indeed, the carrier distribution at the top of a TB or a Schottky barrier is approximately of a hemi-Maxwellian form [12] (in the idealized thermionic model this form is "exact"); deviations result from carriers returning from over the cliff and from the cooling effect). Therefore, the carrier concentration is approximately half of the equilibrium concentration and the electron mean velocity in a given direction $v_{th}$ is approximately twice $v_{rec}$. These factors of 2 cancel in the product defining the Richardson constant.

Distortion of the ideal thermionic transport by the electron cooling effect always results in a lower current because the mean velocity of carriers at the top of the barrier is lower than $v_{th}$.

On the other hand, the current predicted by a drift-diffusion model may either exceed or fall short of the Monte Carlo calculated current, because the neglect of ballistic transport and the velocity overshoot on the downhill slope of the TB may turn out to be more important than neglect of the cooling effect.

The actual electron mean velocity profile, calculated by MC for $V_{app} = 0.8$ V, is presented in Fig. 8. The velocity varies steeply near the top of the barrier, exhibits a pronounced overshoot at the beginning of the downhill slope, and finally attains the saturation value after a distance corresponding to the momentum relaxation time.

Fig. 9 compares the MC simulated current-voltage characteristics of a silicon TB structure with those calculated from the thermionic emission theory. The latter has been applied for low biases only, so as not to violate the condition of nearly flat imref in the uphill region (a fundamental assumption of the thermionic theory [19]). In Table I, the velocity of carriers in the $x$ direction and the concentrations both calculated at the barrier top are compared for the two models at different biases. While the MC concentration is approximately half of the equilibrium concentration, the mean velocity is consistently lower than $v_{th}$, in particular at lower biases and therefore higher retarding fields. These results indicate that the deviation from ideality in the TB manifests itself not so much in the deviation of the imref from...
energy (Fig. 6(b)). The origin of these oscillations can be clearly understood in light of the recent work by Grinberg and Luryi [20], who considered the evolution of an initially cold electronic system interacting with a warmer lattice. Rigorous solution of the kinetic equation shows that in this case the electronic system first rapidly establishes a quasi-equilibrium with optical phonons, and then (after a considerably longer time) the full equilibrium with the lattice is established by the interaction with acoustic phonons. In the quasi-equilibrium state, the electronic system possesses a number of unusual properties, such as a lower mean kinetic energy, suppressed specific heat, and higher acoustic-scattering-limited mobility [20]. The oscillatory quasi-equilibrium distribution is characterized by a definite temperature that is equal to the lattice temperature in the sense that the ratio between the peaks is given by the Boltzmann factor. However, the shape of these peaks “remembers” the initial shape of the cold-electron distribution function due to the nonergodic nature of the interaction with monochromatic optical phonons. Although these properties were established [20] for a nonstationary evolution of a uniform electron system, while in the present work they are demonstrated in the analysis of a steady-state transport in a nonuniform structure, their nature is clearly the same.

V. CONCLUSIONS AND DISCUSSION

We have performed a Monte Carlo simulation of carrier transport across a semiconductor triangular barrier device. A striking new result is the observation of oscillations in the electron mean kinetic energy as a function of the position along the uphill slope of the barrier when a current flows through the device. These oscillations are shown to be due to the nonequilibrium dynamics of the electron interaction with optical phonons in the situation when other inelastic electron scattering processes are negligible. The energy oscillations are superimposed on a smooth cooling of the distribution in the direction of the imposed electric field and show a behavior that is due to the Boltzmann distribution theory.

The energy oscillations discovered in this work manifest a peculiar order that exists in the short-range transport in semiconductors. This order is associated with the fact that all inelastic scattering processes by far most effective is the interaction with the field of dispersionless optical phonons. That leaves a range in both the spatial and temporal domains in which those other inelastic processes can be neglected in the calculation of important transport characteristics. This range defines a mesoscopic scale in the classical transport that is of particular interest because it often extends over the entire size of modern semiconductor devices.

An order parameter, associated with this mesoscopic scale, was recently introduced [21] in connection with the current oscillations in heterojunction tunnel-barrier diodes. That parameter, the reduced differential current (RDC), is a vector field and a function of the electron energy. It is approximately conserved in the mesoscopic transport. Although it is possible to discuss our present results in terms of the RDC, we chose not to do so because the Monte Carlo method allows a more direct analysis of the situation. On the other hand, recent investigation [22] of the range of validity of the RDC conservation, based on a rigorous analysis of the Boltzmann kinetic equation, quanti-
flies the scale of the relevant mesoscopic order. In the absence of electron-electron scattering, degradation of this order occurs mainly because of the inelastic acoustic-phonon scattering, as demonstrated in the present work. At higher temperatures, the degradation can also result from the dispersion in the optical phonon energy. In GaAs the mesoscopic regime extends over larger distances than in Si, mainly because of the lower effective electronic mass [22].

It should be clearly understood that the mesoscopic transport order is a single-electron property not conserved under interelectronic interaction. The triangular barrier structure, where the carrier density is low in the active device region and the electron-electron scattering unimportant, is, therefore, an ideal object of study in this regard.

It should be also noted that observable manifestations of the mesoscopic order may involve some form of spatial averaging which in some cases can wash out the structure induced by optical phonons. For example, although the periodic structure in the distribution function is a true local property unaffected by any form of elastic scattering, the phase of the oscillations relative to the bottom of the conduction band fluctuates together with the electrostatic potential due to discrete impurities [23]. Averaging over these random phases can smear out the oscillatory structure. However, not every experimental situation calls for such an averaging: an example where the mesoscopic order gives rise to observable manifestations is provided by the Hickmott experiment, analyzed in [21].

REFERENCES


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