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A model for the current instabilities in GaAs-AlGaAs heterojunction

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A model is proposed for the description of the current instabilities in GaAs-AlGaAs heterojunctions. It consists of three parts: the injection of electrons via the contact into the AlGaAs layer, the partial capture of these electrons in deep centers, and the change with time of the band structure. This last ingredient is crucial, since due to the increase of the total number of electrons in the AlGaAs layer the band bending decreases making real-space transfer from the AlGaAs layer to the two-dimensional electron gas possible. We have performed quasistationary simulations of the time dependence of the current. The velocities, average energies, capture rates, etc. were taken from Monte Carlo simulations. It turned out, that the parameters for the modeling of the contact, which are to a high degree unknown, play an essential role. © *1996 American Institute of Physics*. [S0021-8979(96)02104-5]

I. INTRODUCTION

In a number of experiments on hot electrons in GaAs-AlGaAs heterojunctions current irregularities have been found. These phenomena have received widespread attention because of the consequences for applications.¹ Especially the groups in Sussex^{2–4} and Eindhoven^{5–7} have paid much attention to these effects. Most of the experiments are I-V measurements, where a high-voltage pulse is applied to a twoterminal device. A variety of phenomena have been observed viz. oscillations, jumps, current filamentation, etc. Various, sometimes only qualitative, explanations have been proposed, most of them containing some *ad hoc* assumptions such as, e.g., real-space transfer out of the two-dimensional electron gas (2DEG) or sudden ionization of electrons captured by deep traps, but no consistent description has been developed until now.

In this paper we describe the modification of a previous model,⁵ with which we perform quantitative calculations of the time dependence of the current in a heterojunction. We focus on the experiments of Zwaal *et al.*^{6,7} As we will argue the time scales involved justify a quasistationary approach.

This paper has been organized as follows. In Sec. II we describe our model and the algorithm for the simulation of the time-dependent current in a heterojunction under high-field conditions. Since we deal with the capture of hot electrons by deep centers in the AlGaAs, we then proceed with a description of this process in Sec. III. This has been achieved by incorporating capture as a one-step mechanism in a standard Monte Carlo simulation. In Sec. IV we describe and discuss our results of the device simulation. We end with some conclusions.

II. DEVICE SIMULATION: MODEL AND METHOD

Before we start with the description of our model it is worthwhile to look at the time scales involved. It is well known from Monte Carlo simulations that the internal settling time of an electron gas is in the order of ps. This time is much smaller than the transit time (ns) through samples with a length of μ m as used in the experiments of Zwaal *et al.*⁶ This time again differs some orders of magnitudes from the rise time of the current jumps found experimentally (μ s). So we deal with an almost quasistationary problem. In such circumstances one can use for the local drift velocity, capture rate etc. the equilibrium values at the appropriate field, concentration and temperature. These values can be obtained from standard Monte Carlo simulations such as to be described in the next section. In this respect our approach can be characterized as hybrid.

When we inspect the typical geometry of the samples used, we notice, that the distance between the 2DEG and the electrons in the AlGaAs is on the order of 100 Å, whereas the samples have lengths of 10 μ m or more. As a consequence, also following from the quasistationary approximation we have to require strict charge neutrality perpendicular to the current flow. In formula with an obvious notation (*x*: coordinate along the field, carrier concentrations, etc. integrated along growth direction)

$$n^{2\mathrm{D}}(x,t) + n^{\mathrm{AlGaAs}}(x,t) = n^{\mathrm{DON}}(x,t) = n^{\mathrm{DON}}(x,0) - n^{\mathrm{CAP}}(x,t)$$
(1a)

or

$$n^{\text{2D}}(x,t) + n^{\text{CAPT}}(x,t) = n^{\text{AlGaAs}}(x,t) = n^{\text{2D}}(x,t=0)\{x,t\}.$$
(1b)

Relaxing this condition would induce very strong electric fields, which restore the charge neutrality on a fs time scale.⁸ By this Eq. (1) the processes in the 2DEG and in the AlGaAs are coupled. The captured and free electrons in the AlGaAs act as a gate, which eventually pinches off the 2DEG channel.

We now make a major assumption: we assume that the situation in the AlGaAs dominates and that the 2DEG adapts itself according to the charge neutrality condition of Eqs. (1a) and (1b). For this we have the following arguments. Due to the low position of the *L* and *X* valleys in AlGaAs (30% Al), there will be a sizeable occupation of these valleys, even at low fields. Thus the overall effective mass in the AlGaAs is (much) larger than in the 2DEG. Furthermore, the mobility

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FIG. 1. The various contributions to the charge distribution in heterojunction as a function of the position parallel to the interface.

in the AlGaAs is very low as a consequence of the random alloy scattering and the high concentration of ionized impurities. So the 2DEG can adapt itself much faster to a changing situation than the electrons in the AlGaAs. This situation resembles the one in an electron-(heavy)hole plasma.

In our simulation we have to discretize in space and time. The spatial grid had a width of $\Delta x = 0.1 \ \mu$ m. The timesteps Δt are coupled to Δx by

$$\Delta x = V^{3\mathrm{D}} \cdot \Delta t. \tag{2}$$

Here V^{3D} is the velocity in the AlGaAs. This gives a timestep of 50–100 ps, large enough to warrant internal equilibrium inside each spatial bin. So we arrive at the following transport algorithm:

capture: $n_k^3(t+\Delta t) = n_k^3(t) - \alpha n_k^3(t)N_k(t)\Delta t$, $N_k(t+\Delta t) = N_k(t) - \alpha n_k^3(t)N_k(t)\Delta t$; drift: $n_{k+1}^3(t+\Delta t) = n_k^3(t+\Delta t)$, $n_1^3(t+\Delta t) =$ injection; neutrality: $n_k^2(t+\Delta t) = N_k(t+\Delta t) - n_k^3(t+\Delta t)$.

Here we use the notation of
$$n^2$$
 for the 2DEG, n^3 for the free
electrons in the AlGaAs, and N for the empty capture cen-
ters. All these concentrations are integrated over the spatial
bin. The index k symbolizes the discretized position x. The

bin. The index k symbolizes the discretized position x. The capture rate is given by α . The number of captured electrons n^{CAP} follows immediately:

$$n_{k}^{\text{CAP}}(t) = N_{k}(t=0) - N_{k}(t).$$
(4)

The current through the device consists of various distributions. First, we have the current flowing in the AlGaAs layer, which is simply the charge in the last bin (k0) divided by Δt :

$$I^{3}(t+\Delta t) = e n_{k0}^{3}(t) / \Delta t.$$
(5)

Next we have the current flowing through the 2DEG. This is somewhat complicated. To elucidate this we inspect the sche-



FIG. 2. The transition region between the contact and the AlGaAs layer as seen parallel to the interface. The electron gas in the metallic contact is indicated by its Fermi–Dirac distribution.

matic diagram in Fig. 1, where for the sake of clarity the features have been exaggerated as compared with a real simulation. It is clear that not all the electrons in the 2DEG are free to drift with their unperturbed velocity, which would give an expression analogous to Eq. (5). We can (artificially) divide the 2DEG in two parts: a part with a position-independent concentration n_{\min}^2 (for the definition see Fig. 1) and a position-dependent rest. The first part moves unhindered giving a contribution of:

$$I^{2}(t + \Delta t) = e n_{\min}^{2}(t) / \Delta t \ V^{2D} / V^{3D}.$$
 (6)

The rest of the 2DEG electrons are fixed to their position according to the requirement of charge neutrality. They only give a current contribution arising from the decrease of the total number of electrons in the 2DEG. Since this decrease is very slow, this contribution is negligible, except as a transient at the beginning of the voltage pulse.

An uncertain part in our model is the injection from the contact into the AlGaAs layer. We consider the contact as a kind of metal containing a free-electron gas with effective mass $m^* = 1.0$ (see Figs. 2 and 3). The concentration was used as a free parameter with values between 10^{19} and 10^{20} cm⁻³.

A very important parameter is the width W of the transition layer between the contact and the AlGaAs layer (Fig. 2). When we apply a voltage, the barrier between the contact and the AlGaAs will be lowered; the larger W the lower the



FIG. 3. Cross section of the heterojunction perpendicular to the interface during the application of a voltage pulse. Indicated are the electron gas in the contact, the 2DEG, the electrons injected in then AlGaAs layer, the positive (+) and by captured neutralized (0) deep centers. An important feature is the lowering of the barrier *B* for the real-space transfer from the AlGaAs into the 2DEG.

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(3)

barrier and the larger the injected current. In practice we only have thermionic injection, the effective width of the barrier being too large for a significant contribution of tunneling.

Another parameter is the distance ΔE of the Fermi level in the contact below the minimum of the conduction band in the AlGaAs. When we inject electrons into the AlGaAs, this distance will increase due to three effects. First, the triangular well widens resulting in a lower energy of the bound state. Next, the Fermi level in the 2DEG decreases. Finally, the band bending in the AlGaAs decreases causing the triangular well as a whole going down. All these effects are illustrated in Fig. 3. In our calculations we accounted for these effects by adjusting ΔE continuously according to the status of the first bin. Thus the initial value of ΔE is not critical, because an equilibrium is established, provided there is some injection.

An important aspect in this game is the decrease of the band bending, which results in a lowering of the barrier B(see Fig. 3) for the transfer of electrons from the AlGaAs into the 2DEG. We think that this phenomenon is responsible for the current jumps found experimentally,⁶ because the slow electrons become fast again. We have schematically modeled this real-space transfer (RST) as follows. If the barrier B at a position k is lower than a certain threshold, we transfer all the electrons in this bin from the AlGaAs to the 2DEG. This threshold depends on the average energy, which we take from a bulk Monte Carlo simulation in AlGaAs. This procedure of course will cause sharp jumps. In reality these jumps are quite smooth, while only a part of the electrons is being transferred, a part, however, which is increasing in time. Under normal conditions this real-space transfer will take place at the source, since the decreasing of the band bending is the strongest over there. We then have a short circuit at the source and also the injected current is flowing through the 2DEG channel. It should be noted, that this RST is in a direction opposite to the one assumed usually.⁴

III. MONTE CARLO SIMULATION OF CAPTURE

In our transport equations appears an overall capture rate α , which may depend on various conditions. The model we used for the calculation of this quantity is based on the work of Mooney *et al.*⁹ We start from the rate equation

$$dn(E)/dt = -K \ n(E) \ N(E), \tag{7}$$

where n(E) and N(E) are the number of electrons and capture states, respectively, at an energy E. In the model of Mooney the capture states are assumed to be concentrated around an energy E_B within an interval δE . In this case the capture probability K can be taken energy independent due to the concentration of the capture states in a narrow energy region.

This single-electron model is a simple description of a quite complicated process. It is nowadays accepted generally, that a Si atom is displaced from a lattice site to an interstitial state, where it is bound due to the presence of an extra electron. The energy E_B is now interpreted as the height of the barrier for the Si atom between the two positions. The real situation, however, may even by more complicated. Among others Theis and Mooney¹⁰ and Jantsch *et al.*¹¹ have argued,

that the capture process proceeds in two steps. One electron is captured by a positive donor to a neutral intermediate state, which in turn captures a second electron forming the famous DX^- center.

The value of 40 meV for the interval δE strongly suggests, that a LO phonon is involved. Moreover, it is well known that the electron lattice interaction via the LO phonons is very strong. We therefore assume that the electron is captured while emitting a LO phonon. This induces an intrinsic temperature dependence in the capture coefficient *K*, which can now be written as

$$K = M_0(N_q + 1)$$
 (8)

in which M_0 is the microscopic transition probability and N_q is the phonon occupation number. Due to the high momenta involved we have, following Theis and Mooney,¹⁰ restricted the capture to electrons in the *L* or *X* valley, which have crystal momenta near the end of the Brillouin zone. The LO phonon now takes care of the conservation of momentum. Relaxing the restriction of the capture to the *L* and *X* valleys hardly changes the results, since there are only a few electrons in the Γ valley at E_B due to the very efficient intervalley scattering.

The model ascribed above has been incorporated in a standard Monte Carlo simulation code.¹² All relevant scattering mechanisms such as acoustic and optical phonon, ionized impurity, random alloy, and intervalley scattering¹³ have been included. We used the simple Debye screening. The various parameters have been taken from the review paper by Adachi,¹⁴ from which we also derived the position of the satellite valleys.

The results of our calculations are presented as an overall capture rate α defined by

$$dn/dt = -\alpha n N/N_0. \tag{9}$$

We have normalized our results to a total number of capture centra N_0 of 10^{18} cm⁻³. So α is average over the capture probability of Eq. (7) and may depend on field, temperature, and concentration.

We start with calculating the field and temperature dependence of the capture rate α , while keeping the electron concentration constant at 0.5×10^{18} cm⁻³. For the capture coefficient *K* we used a value of 10^{-11} cm³ s⁻¹ at 300 K, with a temperature dependence given by Eq. (8).

The results are given in Fig. 4. It is clear that we can distinguish two different regimes. Above 110 K we see a capture, which is almost independent of the field and which decreases exponentially with decreasing temperature. The slopes of the curves give an activation energy of about 110 meV. This is just the energy of the barrier above the bottom of the *L* and *X* valleys. An electron can obtain this energy by three successive absorptions of an optical phonon. The relative probability of this process as compared with emission is $(N_q/2N_q + 1)^3$, which factor gives the desired temperature dependence. Also the inspection of the distribution function learns, that it is a maxwellian with the electron temperature nearly equal to the lattice temperature.

Below 100 K we can discern a growing influence of the electric field, which now becomes more and more respon-

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FIG. 4. The calculated capture rate as a function of the temperature for various electric fields (a) 10 kV/cm, (b) 7.5 kV/cm, and (c) 5 kV/cm.

sible for the heating of the electrons. The distribution becomes more or less temperature independent, giving a constant capture rate. This is due to the decreasing importance of phonon scattering as an energy dissipating mechanism.

Next we calculated the dependence on the electron concentration (see Fig. 5). At high temperatures the capture rate is constant, an immediate consequence of the maxwellian distribution function. At low temperatures the distribution function is more Fermi–Dirac like. When the concentration is low, the Fermi level is well below the capture region resulting in a much lower capture rate.

The only experimental data we can compare with are the results of Theis and Parker.¹⁵ These authors have measured the decay of the conductivity for various fields ranging from 3 to 5 kV/cm. They give the time for a reduction to 95% of the original value. This quantity is not directly comparable with our capture rate, since the capture rate as well as the mobility may depend on the concentration. Nevertheless, the overall features, an exponential decay at high temperatures and a nearly constant value at low *T*, are exactly the same. Even there is an indication for an increase at very low temperatures. The activation energy of 103 meV corresponds surprisingly well with the value extracted from our calculations. This corroborates the value of 180 meV used for the barrier height E_B .

This only (possible) disagreement between experiment and theoretical calculations is the field dependence at low temperatures. The calculations predict a stronger dependence than found experimentally. Moreover, Monte Carlo calculations show that the velocity decreases with carrier concentration making the situation even worse.

The explanation of this discrepancy may be the one step approximation of the capture process. This can be explained as follows. Let us assume that the one step process proceeds at an energy E_B with a probability P_0 and that the two successive steps proceed at E_1 and E_2 ($E_1 + E_2 = E_B$) with probabilities P_1 and P_2 . For the one-step process the capture rate is given by $P_0 f(E_B)$, while for the two-step transition



FIG. 5. The calculated capture rate as a function of the carrier concentration. The calculations have been performed at a field of 10 kV/cm for two different temperatures (a) 300 K and (b) 10 K.

the expression $[P_1 f(E_1)][P_2 f(E_2)]$ holds [f(E) is the distribution function]. For high temperatures the two alternatives have the same temperature dependence viz. exp($-E_0/k_BT$). For low temperatures and fields, however, $f(E_0)$ vanishes, while $f(E_1)$ and $f(E_2)$ still have a finite value. Under these conditions the two-step process may dominate still and may give a sizeable capture rate. The incorporation of such a two-step process may be the subject of a future investigation, provided that we can make a reasonable guess of the parameters involved. This incorporation is necessary if we want to extend our device simulations to lower temperatures. It will become clear in the next session, that for these simulations we need a realistic capture rate.

IV. DEVICE SIMULATION: RESULTS AND DISCUSSION

A typical result of a simulation along the lines sketched above is given in Fig. 6, where we have varied some of the contact parameters. We see a very sharp initial decrease of the current to less than 50% of the expected "normal" value as a response on turning on the voltage, followed by a slow decay, after which a current jump occurs. The very first part reflects the injection at the source into the first bin. In practice this will be smoother as one has to average over a certain region. Such a steep decrease followed by a slow decay has been found experimentally.¹⁶ As mentioned in the introduction also current jumps after some microseconds have been reported.⁷ As explained previously in Sec. II due to our algorithm the jumps in Fig. 6 are very sharp, while experimentally they have a rise time in the μ s region. Keeping this in mind we can speak of a good agreement between theory and experiment.

It is also clear, that especially the width of the transition layer (W see Fig. 2) is of crucial importance. This can easily be understood. If W is large, the barrier is lowered drastically

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FIG. 6. The current response of a heterojunction as a function of time during the application of a block pulse of 1 kV/cm at T = 300 K. The calculations have been performed for two different values of the transition region W between contact and AlGaAs and for two different electron concentrations in the contact. (a) $W = 0.30 \,\mu$ s, $n = 10^{20} \,\mathrm{cm}^{-3}$; (b) $W = 0.30 \,\mu$ s, $n = 10^{19} \,\mathrm{cm}^{-3}$; (c) $W = 0.02 \,\mu$ s, $n = 10^{20} \,\mathrm{cm}^{-3}$; (d) $W = 0.02 \,\mu$ s, $n = 10^{19} \,\mathrm{cm}^{-3}$.

and we have a strong injection. Under these circumstances the majority of the electrons in the AlGaAs are free (see Fig. 1). The threshold for real-space transfer will be reached relatively early and a large jump will occur.

The influence of the electric field manifests itself in a twofold way. First, the barrier for the injection is lowered, resulting in an increase of the electrons in the AlGaAs. On the other hand, the velocity is higher causing the capture to decrease. These two effects work in opposite directions, so at first sight it is not clear, whether the current jumps occur earlier or later, when we increase the field. We have investigated the time of the jumps versus the electric field for the two geometries used in Fig. 6. When we have a good contact (W is small) the jumps occur at a later time, changing the field from 1 to 2 kV/cm shifts the jump from 3.8 to 7.1 μ s. On the other hand, when W is large the jump shifts from 1 to about 0.5 μ s. In the experiment of Zwaal *et al.*⁶ the jumps shift to earlier times with increasing field. Also the appreciable size of the jumps (see Fig. 6) is a strong indication for a large W in the sample used.

We now can understand why filaments can occur and why we sometimes see consecutive jumps, the first one being the largest. If W varies along the contact pad, the injection varies with all consequences. The changes in current profile can be considerable due to the high sensitivity for the precise value of W. There exists convincing evidence for such variations in contact structure.^{17,18}

The calculations presented above have been performed at a temperature of 300 K. The temperature dependence of the time of the current jump has been investigated as well. The result of a temperature decrease is a combination of various effects: (1) The decrease of the capture rate with temperature has an activation energy of 110 meV, so the number of captured electrons diminishes drastically.

(2) Moreover, the velocity in the AlGaAs increases, making Δt smaller, again lowering the capture efficiency.

(3) The tail of the Fermi–Dirac distribution in the contact shrinks with the result of less thermoionic injection.

(4) For not too low temperatures (T > 100 K) the average energy of the electrons is $3/2k_BT$. This implies that the band bending has to decrease more before real-space transfer can occur.

All these effects work in the same direction viz. it lasts longer before a current jump occurs. In our calculations we have found an exponential dependence of the inverse time $(1/\tau_{jump})$ with an activation energy around 300 meV. This value is a result of the combined effects mentioned above, starting with the 100 meV activation energy connected with the capture. It is therefore very surprising that the experiments by Zwaal *et al.*⁷ give a value as low as 80 meV. The origin of this discrepancy is not clear. It might have to do with the possible two-step capture. Another possibility is, that the structure of the transition between contact and AlGaAs is more complicated than in our model, keeping the injection at a high level.

Indications for a more complicated structure can be found in the work of Hendriks *et al.*⁵ These authors found current oscillations at relatively low fields ($\leq 1 \text{ kV/cm}$), indicating a certain bistability. Such bistabilities have been found in double barrier resonant tunneling (DBRT) diodes.¹⁹ If we assume a grain structure at the contact, which is reasonable in view of experimental evidence from transmission electron microscope (TEM) pictures,^{17,18} we may have a DBRT-like band diagram in the transition layer. It is then clear that this can introduce a bistability, which vanishes when a magnetic field is applied.¹⁹

We will end with some remarks on the interpretation of the time-resolved optical beam-induced current (TROBIC) experiments as performed by Zwaal *et al.*⁶ In these experiments one empties the deep centers with a short laser pulse. Unfortunately, also a lot of electron-hole pairs are created, making the situation quite complicated. Strictly speaking our model, which is quasistationary and is based on rigid charge neutrality [see Eq. (1)], may not be applicable in such a suddenly changing situation, where internal fields play a dominant role. It nevertheless provides us with keys for the explanation of the experiments.

Let us suppose that the traps are emptied at a position k and time t. In the next timestep all the free carriers at position k (much more than usual) are transferred to position k + 1. This results in a spike into the 2DEG as schematically depicted in Fig. 7. Starting from this graph we can discern three possibilities. First, the spike remains above the level n_{\min}^2 . There is no additional suppressing of the current in the 2DEG. The effect is a short positive pulse, when the extra carriers reach the drain. This situation will occur in the region of the drain.

Next the spike can give an extra suppression of the 2DEG. This will have a (strong) negative effect on the total

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FIG. 7. As Fig. 1. The situation one timestep after the application of a laser pulse, which ionizes all the deep centers.

current, lasting as long as the spike travels through the sample.

Finally, the sum of captured and free carriers at position k + 1 may exceed the threshold n_{th}^2 for real space transfer to the 2DEG. In our model the transfer is complete. In these circumstances this is much too simple. Probably there is an incomplete transfer and the 2DEG is pinched off to the real-space transfer threshold. The effect will be somewhat less than in the second case.

We may conclude that the proposed model is capable to explain and understand a number of experimentally found phenomena. Since it assumes simple homogeneous material it may provide a good starting point for models in which structural fluctuations such as Al or Si clustering are included.

V. CONCLUSIONS

In summary, we have developed a model for the understanding of current instabilities in GaAs-AlGaAs heterojunctions. It comprises three parts: the injection of electrons into the AlGaAs layer, the capture of these electrons in deep centers, and a time-dependent modification of the band structure making real-space transfer from the AlGaAs to the 2DEG possible. It turned out, that the modeling of the contact is the crucial ingredient. We have shown that for reasonable values for the parameters of the contact, field-induced parallel conduction in the AlGaAs occurs. Once this being established current jumps, filament formation, etc. follow quite naturally. Our model does not contain additional physical assumptions. It therefore provides a good starting point for future investigations, as well experimentally as theoretically. The main uncertainties reside in the modeling of the transition between the metallic contact and the semiconductor. Therefore it might be worthwhile to consider a more sophisticated approach. Nevertheless, in view of all the approximations made, we judge the agreement between experiment and simulations as very satisfactory.

We also incorporated the capture of electrons into deep centra in a standard 3D Monte Carlo simulation. For this we used a one-step model, which probably is too simple. The essential features of the experimental data, however, have been described quite well.

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