
Free boundary problems describing two-dimensional pulse recycling and motion in semiconductors

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Abstract A reduction of the Kroemer's model for the two-dimensional Gunn effect to a free boundary problem (FBP) is presented. The Gunn moving pulse is approximated far from the contacts by a moving free boundary separating regions where the electric potential solves a Laplace equation with subsidiary boundary conditions. We obtain the exact solution in simple one-dimensional and axisymmetric geometries. The agreement is excellent so that the FBP can be adopted as the basis for a general asymptotic study of the multi-dimensional Gunn effect.

1 Introduction

The Gunn effect is a charge transport phenomenon which takes place in semiconductor devices displaying negative differential resistivity in their current-field characteristics. A *dc* voltage bias applied to the sample leads to pulse recycling (at contacts) and motion that give rise to self-sustained oscillations of the electric current. Most of the theoretical and experimental studies deal with one dimensional geometries of samples with attached planar contacts. Recently, experiments [WM94] and numerical and asymptotic studies [BE01, BEH01] have considered cylindrical and rectangular geometries with point contacts. The numerical simulations are based upon the Kroemer's model [Kro66] and, in two-dimensional samples where many unusual oscillatory patterns are found, the computational cost makes inaccessible the analysis of large samples. It is then necessary to find new ideas, such as the formulation of a free boundary problem we present here.

The Kroemer's model consists of the following equations and boundary conditions (in dimensionless units, see, *e.g.*, [HB92] for details) for the concentration of free carriers (electrons), n , and the electric potential, φ :

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v} - \delta \nabla n) = 0, \quad (1)$$

$$\nabla^2 \varphi = n - 1, \quad (2)$$

$$\mathbf{v}(\mathbf{E}) = \mathbf{E} \frac{1 + v_s E^3}{1 + E^4}, \quad (3)$$

$$\mathbf{x} \in \Sigma_c : \mathbf{E} \cdot \mathbf{N} = \rho (n\mathbf{v} - \delta \nabla n) \cdot \mathbf{N} \quad \text{and} \quad \varphi = 0, \quad (4)$$

$$\mathbf{x} \in \Sigma_a : \mathbf{E} \cdot \mathbf{N} = \rho (n\mathbf{v} - \delta \nabla n) \cdot \mathbf{N} \quad \text{and} \quad \varphi = \Phi, \quad (5)$$

$$\mathbf{x} \in \Sigma_o : \mathbf{E} \cdot \mathbf{N} = 0 \quad \text{and} \quad (n\mathbf{v} - \delta \nabla n) \cdot \mathbf{N} = 0. \quad (6)$$

Eqs. (1) and (2) are the charge continuity and Poisson equations, respectively, where $\mathbf{v}(\mathbf{E})$ is the carrier drift velocity and $\mathbf{E} = \nabla \varphi$ is the electric field ($E = |\mathbf{E}|$). We assume $v_s = 0$ and a constant diffusion coefficient: $\delta \approx 0.013$.

Our boundary conditions (4) and (5) at the interfaces between semiconductor and contacts, $\Sigma_{c,a}$, and on the outer boundary of the semiconductor boundary Σ_o assume that the normal components of electron current density and electric field are proportional at the semiconductor–contact boundary (Ohm's law) [HB92] (\mathbf{N} is the unit normal to $\Sigma_{c,a}$ directed towards the semiconductor). For simplicity, we choose all contact resistivities to be equal: $\rho = 2$. Bias conditions are $\varphi = 0$ at the cathode Σ_c (injecting contact) and $\varphi = \Phi$ (the applied voltage) at the anode Σ_a (receiving contact). If part of the semiconductor boundary does not have attached contacts, the corresponding boundary conditions are zero flux ones, as in Eq. (6).

An Ampère's equation can be written for the total current density (electronic plus displacement), \mathbf{j} , by eliminating n from (1) using (2):

$$\begin{aligned} \nabla \cdot \mathbf{j} &= 0, & \text{with} \\ \mathbf{j} &= (1 + \nabla^2 \varphi) \mathbf{v} - \delta \nabla (\nabla^2 \varphi) + \frac{\partial \mathbf{E}}{\partial t}. \end{aligned} \quad (7)$$

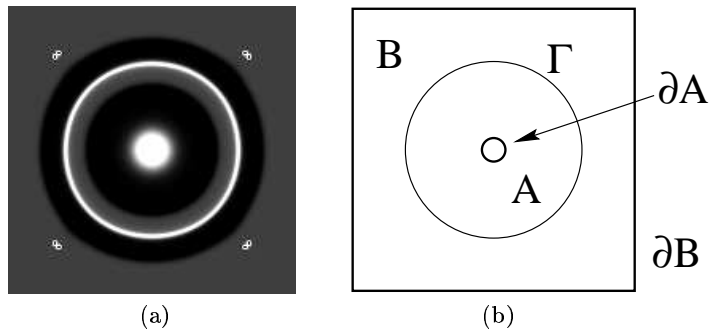


Fig. 1. Approximation of the Gunn moving pulse (a) obtained with direct numerical simulations of the Kroemer's model by a moving free boundary Γ separating the sample in two regions A and B (b) in which φ solves the Laplace equation.

2 The Free Boundary Problem

It is known from [BEH01] that outside the wave the field is small and $v(E) \approx E$ except near the contacts and inside pulses. There, space and time derivatives can be neglected in Eq. (7), which implies $\mathbf{j} \approx \mathbf{E}$ and the electric potential φ is a harmonic function outside pulses and contact regions: $\nabla^2 \varphi = 0$.

The pulse is a narrow region of high electric field made of a leading front and a trailing front which is a shock wave with speed $V \sim \pi/(4E_+)$ given by the equal area rule, where E_+ is the height of the wave [BEH01]. The leading front is a region at which $n = 1 + \nabla \cdot \mathbf{E} \approx 0$. Far from the contacts the electric field is normal to the pulse and the velocity of the leading front is $j_N = \mathbf{j} \cdot \mathbf{N}$.

A key observation is that the pulse is *narrow* and it can be substituted by a curve on a length scale of the order of the distance between contacts, L . See Fig. 1. We shall assume that its width remains much smaller than L so that the pulse is a curve Γ given by the equation: $W(\mathbf{x}, t) = 0$.

Clearly, there is a finite voltage drop across the pulse, $\sim E_+^2/2 = O(\Phi)$, which means that the electric potential has a jump discontinuity at Γ : $E_+^2/2 = [\varphi] \equiv \varphi_+ - \varphi_-$. Here φ_- and φ_+ are the limiting values of φ as \mathbf{x} approaches Γ from the region inside or outside Γ , respectively. The relations $\text{div} \mathbf{j} = 0$ and $\mathbf{j} \approx \mathbf{E}$ imply that the normal component of the electric field (and therefore the normal derivative of the electric potential) is continuous across Γ :

$$j_N = (\mathbf{N} \cdot \nabla \varphi)_+ = (\mathbf{N} \cdot \nabla \varphi)_-. \quad (8)$$

This j_N is also the velocity of the leading front of the pulse along its normal, which is nearly equal to that of the trailing front, V , during most of the pulse lifetime. The pulse velocity can also be obtained by differentiating $W(\mathbf{x}, t) = 0$ with respect to time: $W_t + \nabla W \cdot (d\mathbf{x}/dt) = 0$. Since $\mathbf{N} = \nabla W / |\nabla W|$, the normal component of the pulse velocity, j_N , is

$$\frac{d\mathbf{x}}{dt} \cdot \mathbf{N} = -\frac{1}{|\nabla W|} W_t. \quad (9)$$

Then, using $V = \pi/(4E_+)$ and $j_N = V$, we obtain the Hamilton-Jacobi equation (HJE) for the position of Γ which completes the formulation of the FBP:

The electric potential $\varphi(\mathbf{x}, t)$ is a harmonic function inside and outside the free boundary Γ , with boundary conditions (4), (5) and (6) on the semiconductor boundaries. On the free boundary Γ , implicitly given by $W(\mathbf{x}, t) = 0$, φ has a jump discontinuity $[\varphi]$ and its normal derivative satisfies

$$(\mathbf{N} \cdot \nabla \varphi)_+ = \frac{\pi}{4\sqrt{2}[\varphi]} = (\mathbf{N} \cdot \nabla \varphi)_-, \quad (10)$$

where $\mathbf{N} = \nabla W / |\nabla W|$. Furthermore, the free boundary obeys the following Hamilton-Jacobi equation:

$$-W_t = \frac{\pi|\nabla W|}{4\sqrt{2}[\varphi]} \quad \text{on} \quad W(\mathbf{x}, t) = 0. \quad (11)$$

The conditions on the normal derivative of the electric potential at the free boundary are equivalent to:

$$(\nabla\varphi \cdot \nabla W)_+ = \frac{\pi|\nabla W|}{4\sqrt{2}[\varphi]} = (\nabla\varphi \cdot \nabla W)_- \quad \text{on } W(\mathbf{x}, t) = 0. \quad (12)$$

3 Exact Solution in simple geometries

The HJE (11) can be solved by the method of characteristics (the Hamilton equations). To derive them, we just take a partial derivative of the HJE with respect to x , and a partial derivative with respect to y . The results are

$$W_{xt} + \frac{\pi}{4|\nabla W|\sqrt{2}[\varphi]} (W_x W_{xx} + W_y W_{xy}) = \frac{\pi}{8\sqrt{2}[\varphi]^3} [\varphi]_x |\nabla W|,$$

and a similar equation for W_y . The characteristic equations for these first-order quasilinear partial differential equations for $p = W_x$ and $q = W_y$ are

$$\frac{dx}{dt} = \frac{a}{\sqrt{p^2 + q^2}} p, \quad \frac{dy}{dt} = \frac{a}{\sqrt{p^2 + q^2}} q, \quad (13)$$

$$\frac{dp}{dt} = -\frac{a}{2[\varphi]} [\varphi]_s q, \quad \frac{dq}{dt} = \frac{a}{2[\varphi]} [\varphi]_s p, \quad (14)$$

$a = \pi/(4\sqrt{2}[\varphi])$, together with $W_t = 0$, which follows from the chain rule:

$$\frac{dW}{dt} = W_t + W_x \frac{dx}{dt} + W_y \frac{dy}{dt} = W_t + a|\nabla W| = 0. \quad (15)$$

In the four equations (13)-(14), s is arc length on Γ , and we have used that $[\varphi]_x = -q[\varphi]_s/\sqrt{p^2 + q^2}$ and $[\varphi]_y = p[\varphi]_s/\sqrt{p^2 + q^2}$ on Γ . These expressions can be derived by using a local coordinate system on Γ with basis vectors $\mathbf{N} = \nabla W/|\nabla W|$ and $\mathbf{T} = (-W_y, W_x)/|\nabla W|$. The jump $[\varphi]$ depends only on the arc length on Γ and t because it is defined only for $(x, y) \in \Gamma$ [these $(x, y) \in \Gamma$ have zero projection onto \mathbf{N}].

The FBP can be solved exactly in two simple geometries: a rectangular sample with planar contacts attached at the ends (1D case), and the Corbino geometry of two concentric circular contacts (axisymmetric case, as in Fig. 1).

In the 1D case the electric potential depends only on x , the cathode is located at $x = 0$, the anode at $x = L$, and the FB is a moving point $x_s(t)$. The solutions are $\varphi_A(x, t) = ax$ in $[0, x_s]$ and $\varphi_B(x, t) = a(x - L) + \Phi$ in $[x_s, L]$. The jump $[\varphi] = \varphi_B(x_s, t) - \varphi_A(x_s, t)$ solves the equation $[\varphi] = \Phi - aL$, i.e. $\alpha^3 = \phi\alpha - aL$, where $\alpha = \sqrt{[\varphi]}$; it is independent of t and x_s . When there are two positive solutions, it can be shown that the pulse with smaller $[\varphi]$ is unstable. Then $x_s(t)$ can be found by solving $-W_t = a|W_x|$, whose solution is: $W(x, t) = W_0(x - at)$. Then $x_s(t) = x_s(0) + at$. See Fig. 2(A).

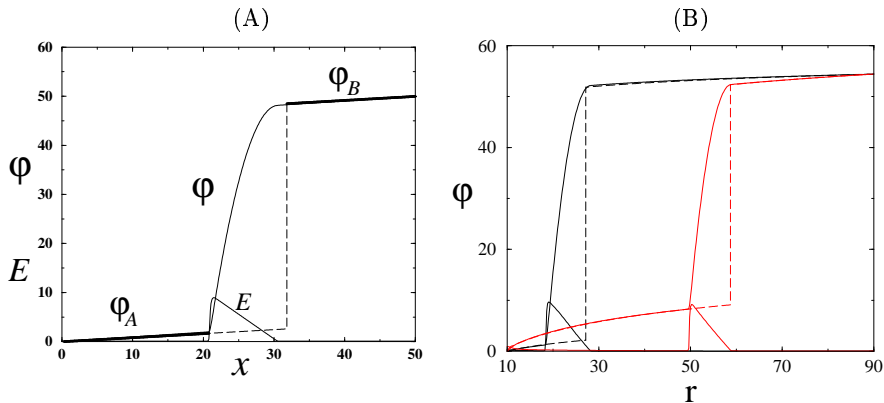


Fig. 2. Electric potential and field (solid lines) of an advancing pulse (far from the contacts) calculated by numerically solving the Kroemer model. (A) 1D and (B) axisymmetric case. They agree very well with the approximations $\varphi_A(x, t)$ and $\varphi_B(x, t)$ (dashed lines), and with the velocity of the free boundary, as shown in (B).

The FBP has yielded the same approximation to the complete 1D problem as indicated in Ref. [HB92] for the motion of a pulse far from the boundaries.

In the axisymmetric case, $\varphi \equiv \varphi(r, t)$ with r measured from the center of the cathode. The solution of $[r\varphi_r]_r = 0$ at both sides of $r_s(t)$ is $\varphi_A(r, t) = ar_s \log(r/r_c)$ and $\varphi_B(r, t) = ar_s \log(r/r_a) + \Phi$, where $r_{c,a}$ are the radii of the contacts. The jump $[\varphi] = \Phi - ar_s \log(r_a/r_c)$ decreases as the pulse advances (cf. [BEH01]). It must be solved simultaneously with the HJE, which yields

$$r_s(t) = r_s(0) + \frac{\pi}{4\sqrt{2}} \int_0^t [\varphi]^{-\frac{1}{2}} dt. \quad (16)$$

Fig. 2(B) shows the perfect agreement with direct numerical simulations of the Kroemer's model, included the velocity of the pulse (see Ref. [BEH01] for a fuller description of self-oscillations in this case).

It is expected that the great reduction in computational cost allowed by using the FBP as an alternative to solving the full Kroemer model would enable us to study much larger samples in multi-dimensional geometries.

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