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Cite as: Appl. Phys. Lett. **76**, 891 (2000); <https://doi.org/10.1063/1.125620>

Submitted: 07 September 1999 • Accepted: 24 November 1999 • Published Online: 04 February 2000

Griff L. Bilbro and Robert J. Nemanich



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# Nongeometric field enhancement in semiconducting cold cathodes and in metal–insulator–semiconductor structures

Griff L. Bilbro

*Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina 27695-7911*

Robert J. Nemanich

*Department of Physics, North Carolina State University, Raleigh, North Carolina 27695-8202*

(Received 7 September 1999; accepted for publication 24 November 1999)

We extend the usual one-dimensional equilibrium theory of the surface space charge region that screens a semiconductor from an external electric field in order to admit perturbations in three dimensions and time. We identify a class of perturbations of the one-dimensional equilibrium that grow exponentially in time at least until our first-order perturbation theory fails. The resulting spontaneous field enhancement may explain enhancement factors observed in electron emission from semiconducting cathodes and may similarly contribute to gate leakage in metal–oxide–semiconductor field effect transistors. © 2000 American Institute of Physics.

[S0003-6951(00)04204-2]

Advanced growth techniques for crystalline films of wide band gap semiconductors with low electron affinity (LEA) may lead to the next generation of cold cathodes.<sup>1</sup> LEA materials may improve field emission arrays and may enable single crystal planar cold cathodes. Calculations indicate that graded  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  LEA films without doping might emit high current densities robustly.<sup>2</sup> Recent calculations indicate that doping might dramatically reduce the operating voltages of such cathodes<sup>3</sup> or the operating temperatures of similar thermionic cathodes.<sup>4</sup>

Emission from sharp cold cathodes is increased by geometric field enhancement, but emission from smooth cold cathodes is also difficult to explain without some mechanism of field enhancement.<sup>5</sup> In addition, low-voltage emission from high quality nitrogen-doped diamond films appears to be preceded by arcing which forms craters in the film, but these craters do not appear sharp enough to account for the improved emission by geometric field enhancement.<sup>5</sup>

Consider the quasiequilibrium states of an ideal planar cold cathode comprising a uniform  $n$ -type semiconductor that fills the half space  $z < 0$ . The electron density is

$$n = N_C \exp\left(\frac{E_{Fn} - E_C}{k_B T}\right)$$

for  $z < 0$ , where  $N_C$  is the effective density of states of the conduction band and the quasi-Fermi level for electrons  $E_{Fn}$  differs from the bulk equilibrium Fermi level by

$$\phi = \frac{E_{Fn} - E_F}{q},$$

measured in volts. The bulk Fermi level is

$$E_F = E_C - k_B T \exp\left(\frac{N_C}{N_D}\right),$$

where  $N_D$  is the density of donors, which are assumed to be completely ionized, and the minimum of the conduction band  $E_C$  can be defined to be zero at  $z = -\infty$  so that

$$\psi = -\frac{E_C}{q}$$

is the usual electric potential in volts. Then

$$n = N_D \exp\left(\frac{\phi + \psi}{V_{th}}\right),$$

where  $V_{th} = k_B T / q$  is the usual thermal voltage. For  $\psi > 0$  the deviations  $\psi$  and  $\phi$  obey Poisson's equation

$$\nabla^2 \psi = -\frac{q}{\epsilon_s} (N_D - n) = \frac{q N_D}{\epsilon_s} \left[ \exp\left(\frac{\psi + \phi}{V_{th}}\right) - 1 \right], \quad (1)$$

in standard units where  $\epsilon_s$  is the dielectric permittivity of the semiconductor and  $q > 0$  is the fundamental charge. The deviations also conserve charge

$$-q \frac{\partial n}{\partial t} + \nabla \cdot \vec{J} = 0, \quad (2)$$

where the current density due to drift and diffusion is

$$\vec{J} = q \mu n \vec{F} + q D \nabla n,$$

and where the electron mobility  $\mu$  and the diffusion coefficient  $D = \mu / V_{th}$  are treated as independent of electric field

$$\vec{F} = -\nabla \psi.$$

Substituting  $\vec{F}$  and

$$\nabla n = \frac{n}{V_{th}} (\nabla \phi + \nabla \psi)$$

into the two contributions for the current simplifies the expression for total current

$$\vec{J} = q \mu n \nabla \phi$$

so that

$$\nabla \cdot \vec{J} = q \mu (n \nabla^2 \phi + \nabla n \cdot \nabla \phi)$$

and Eq. (2) can be written

$$\mu V_{th} \left[ \nabla^2 \phi + \frac{\nabla(\psi + \phi)}{V_{th}} \cdot \nabla \phi \right] = \frac{\partial(\psi + \phi)}{\partial t}$$

in standard units. However, it is convenient to measure lengths and times in units of the extrinsic Debye length and the dielectric relaxation time for electrons in the bulk

$$L_D = \sqrt{\frac{\epsilon_s V_{th}}{q N_D}} \quad \text{and} \quad \tau_R = \frac{\epsilon_s}{q \mu N_D},$$

and to measure voltages in units of the thermal voltage  $V_{th}$ , so that Eqs. (1) and (2) become

$$\nabla^2 \psi = \exp(\psi + \phi) - 1 \quad (3)$$

and

$$\nabla^2 \phi + \nabla(\psi + \phi) \cdot \nabla \phi = \frac{\partial(\psi + \phi)}{\partial t}. \quad (4)$$

We now use Eqs. (3) and (4) to analyze the stability of the electron space charge layer that accumulates near the surface when the semiconductor-vacuum interface is held at a constant voltage  $V_0 > 0$ . We write the electric potential as a zeroth order equilibrium part  $\psi_0$  plus a perturbation

$$\psi = \psi_0(z) + \delta\psi(x, y, z, t).$$

The quasi-Fermi level coincides with the bulk  $E_F$  for any equilibrium state regardless of its stability, so

$$\phi = \delta\phi(x, y, z, t)$$

contains no zeroth order part. Substituting these expressions into Eqs. (3) and (4) yield a zeroth order equation for the usual one-dimensional equilibrium

$$\nabla^2 \psi_0 = e^{\psi_0} - 1 \quad (5)$$

and a pair of equations for the first order dynamics of the perturbations

$$\nabla^2 \delta\psi = e^{\psi_0} (\delta\phi + \delta\psi), \quad (6)$$

$$\nabla^2 \delta\phi + \nabla \psi_0 \cdot \nabla \delta\phi = \frac{\partial(\delta\phi + \delta\psi)}{\partial t}. \quad (7)$$

For  $z \leq 0$ , where  $\psi_0 = 0$  and there is no nearby boundary,  $\delta\phi, \delta\psi \propto \exp(ik_x x + ik_y y + ik_z z + st)$  solves Eqs. (6) and (7) with the usual result that

$$s = -(1 + k_x^2 + k_y^2 + k_z^2)$$

so that a  $k=0$  perturbation dies out in about one unit of time (i.e.,  $\tau_R$ ) and that higher wave number (i.e., relative to  $L_D^{-1}$ ) disturbances die out faster.

However, near the semiconductor-vacuum interface, the  $z$  dependence is not harmonic for  $V_0 > 0$ . In this case, separation of variables using

$$\delta\psi = A(z) \exp(ik_x x + ik_y y + st),$$

$$\delta\phi = B(z) \exp(ik_x x + ik_y y + st)$$

converts the first order Eqs. (6) and (7) into

$$A'' - k^2 A = e^{\psi_0} (A + B), \quad (8)$$

$$B'' - k^2 B + \psi_0' B' = s(A + B), \quad (9)$$

where prime indicates ordinary differentiation with respect to  $z$  and  $k^2 \equiv k_x^2 + k_y^2$ .

The numerical integration of Eqs. (5), (8), and (9) requires six constants which can be determined from the following choices. The zeroth order electric field just inside the cathode,  $-\psi_0'(0)$ , can be specified as the external field divided by the dielectric constant of the semiconductor assuming there is no surface charge density. In this report, we restrict ourselves to the case of zero emitted current, so that  $B'(0) = 0$  since  $\hat{z} \cdot \vec{J} \propto B'$ ; in addition  $B, \psi_0$  and  $A$  all vanish at  $z = -\infty$  for this case. Finally, at some  $z_0 \leq 0$  we choose  $A(z_0)$  arbitrarily since Eqs. (8) and (9) are linear and homogeneous in  $A$  and  $B$  so that the choice does not affect stability.

The dynamics of the perturbations depend on the zeroth order  $\psi_0$  which we find using the following technique. Since  $\lim_{z \rightarrow -\infty} \psi_0(z) = 0$ , there exists a  $z_0$  such that for all  $z \leq z_0$ , Eq. (5) is arbitrarily close to

$$\nabla^2 \psi_0 = \psi_0,$$

where we have used the small argument expansion of the exponential function. Therefore, in the region  $-\infty < z \leq z_0$ , the solution of Eq. (5) is arbitrarily close to

$$\psi_0(z) = a_0 e^z,$$

for some  $a_0$  and where we have used the fact that  $\psi_0(-\infty) = 0$ . The utility of this result is that  $z_0$  can be chosen to make  $\psi_0'(z_0) = \psi_0(z_0)$  to arbitrary accuracy, which provides two boundary conditions at  $z_0$  in terms of one.

For concreteness, we choose  $n$ -type, Si-doped  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  with  $N_D = 10^{24} \text{ m}^{-3}$  and  $x = 0.5$  so that  $\chi \approx 1 \text{ eV}$ , the donor ionization energy is small, and the dielectric constant  $K \approx 8.75$ , as we have previously inferred from the literature.<sup>4</sup> In this case,  $L_D = 3.55 \text{ nm}$  and  $\tau_R = 0.16 \text{ ps}$  at room temperature. We choose the zeroth order electric field just inside the cathode to be  $-1 \text{ V}/\mu\text{m}$  as should occur in a  $n$ -doped LEA cathode. For the following, a value of  $z_0 = -4$  was used because it yielded results similar to other choices,  $z_0 = -5$  and  $z_0 = -3$ .

Numerically integrating (the unapproximated) Eq. (5) from  $z = z_0$  to  $z = 0$  results in a value of  $\psi_0'(0)$  that can be conveniently adjusted with a one-parameter search to obtain  $-\psi_0'(0) V_{th}/L_D = -1 \text{ V}/\mu\text{m}$  for  $\psi_0'(z_0) = 0.1355 \exp(z_0)$ .

The same technique can be used to reformulate the boundary conditions of the perturbative system. As before  $z_0$  can be chosen to make Eqs. (6) and (7) arbitrarily close to

$$A'' - k^2 A = A + B,$$

$$B'' - k^2 B = s(A + B)$$

for all  $-\infty < z \leq z_0$ . In this asymptotic region, Eqs. (6) and (7) comprise a linear, homogeneous system with constant coefficients so that

$$A(z) = a_1 e^{\alpha z},$$

$$B(z) = b_1 e^{\alpha z},$$

for some  $a_1$  and  $b_1$ , where  $\alpha$  is some positive constant, and where we have used the boundary condition that  $A$  and  $B$  vanish at  $z = -\infty$ . Substitution shows that there are two cases

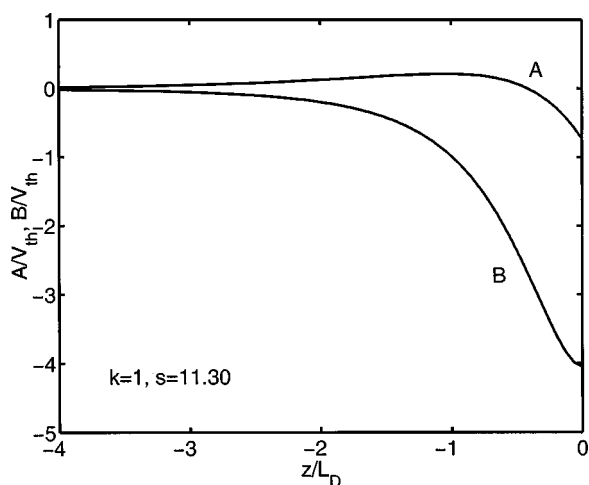


FIG. 1. The perturbation  $A$ ,  $B$  with wave number  $k=1/L_D$  parallel to the semiconductor-insulator interface and exponential growth rate  $s=11.30/\tau_R$ .  $A$  is the deviation of the electric potential from the one-dimensional equilibrium.  $B$  is the deviation of the quasi-Fermi level for electrons from the bulk Fermi level.

- (1)  $\alpha = \sqrt{k^2}$  and  $b_1 = -a_1$ ,
- (2)  $\alpha = \sqrt{s + k^2 + 1}$  and  $b_1 = s a_1$ ,

but in both cases,  $A' = \alpha A$  and  $B' = \alpha B$  in the entire asymptotic region  $-\infty < z \leq z_0$  including  $z = z_0$ . In either case, numerical integration of the (unapproximated) system, Eqs. (8) and (9), from  $z = z_0$  to  $z = 0$  is straightforward with these initial conditions. The second case does not always admit a zero-emission solution, so we address only the first case in this letter.

Determination of  $s$  as a function of  $k$  proceeds as follows. For each  $k$ , an initial value of  $s$  is chosen and the functions  $A$  and  $B$  are numerically integrated from  $z = z_0$  to  $z = 0$  with initial conditions  $A(z_0) = \exp(kz_0)$ ,  $B(z_0) = -A(z_0)$ ,  $A'(z_0) = kA(z_0)$ , and  $B'(z_0) = kB(z_0)$  corresponding to case (1) earlier. The value of  $B'(0)$  is driven to zero by adjusting  $s$  iteratively. For  $k=1$ , for example, the solution  $s=11.30$  is unstable and the resulting functions  $A(z)$  and  $B(z)$  are shown in Fig. 1. In standard units,  $k=0.282 \text{ nm}^{-1}$  and  $s=70.6 \text{ ps}^{-1}$ . The process can be repeated

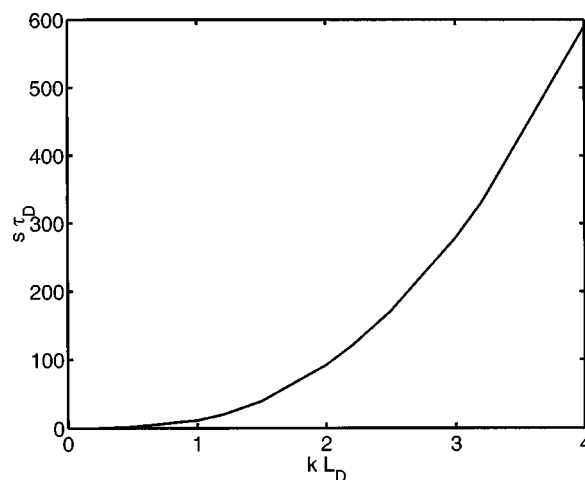


FIG. 2. Growth rate  $s$  vs wave number  $k$  parallel to the semiconductor-insulator interface for the family of perturbations with one finite node in  $A$ , the deviation of the electric potential from the one-dimensional equilibrium.

for several  $k$  to obtain a dispersion relation which shows that the growth rate increases with  $k$  as shown in Fig. 2. Other solutions exist for any  $k$ , for example  $s = -1.97$  is a stable solution for  $k=1$  with no finite nodes in  $A$ .

We conclude that the space charge region that screens a semiconductor from an externally applied electric field is not uniform along the interface, but spontaneously orders itself into regions of higher and lower electron density and electric field, at least before electron emission occurs and while our use of Maxwell Boltzmann statistics is valid.

The analysis is independent of the details of the insulator, so that this conclusion applies to the semiconductor-vacuum interface of cold cathodes and also to the interface between silicon and gate oxide in metal-oxide-semiconductor field effect transistors

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